A Ba-free sealing glass with a high CTE and excellent interface stability optimized for SOFC/SOEC stack applications

A new glass-ceramic composition containing Si, Mg, Ca, Na, Al, Zr and B is presented here as sealant for planar SOFCs/SOECs, with the aim of joining the metallic interconnect (Crofer22APU) to the solid oxide cell (YSZ electrolyte or CGO barrier layer). Characteristic temperature, thermo-mechanical properties and compositional variations are reviewed and discussed by thermal analyses and in situ XRD, in order to design and optimize the sealing profile and reduce the residual porosity. The glass after heat treatment partially devitrifies into augite and nepheline with residual glass phase of around 64.3%; after crystalization the glass-ceramic sealant has a CTE of $12.8 \times 10^{-6} \text{ K}^{-1}$ and it is compliant with the other materials typically used for stack components. This work shows that the developed glass-ceramic can successfully join the ceramic cell with the Crofer22APU (pre-oxidized and alumina coating), proven by tests on small and large-scale samples. No signs of unwanted reactions at the glass-metal and the glass-cell interface are observed and sufficient gas tightness is achieved.

General information

State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Electrofunctional materials, Politecnico di Torino
Authors: Ritucci, I. (Intern), Agersted, K. (Ekstern), Zielke, P. (Intern), Wulff, A. C. (Intern), Khajavi, P. (Intern), Smeacetto, F. (Ekstern), Sabato, A. G. (Ekstern), Kiebach, R. (Intern)
Acid Distribution and Durability of HT-PEM Fuel Cells with Different Electrode Supports

The durability of high-temperature polymer electrolyte membrane fuel cells (HT-PEMFCs) was studied with phosphoric acid doped membranes of polybenzimidazole (PBI). One of the challenges for this technology is the loss and instability of phosphoric acid resulting in performance degradation after long-term operation. The effect of the gas diffusion layers (GDL) on acid loss was studied. Four different commercially available GDLs were subjected to passive ex situ acid uptake by capillary forces and the acid distribution mapped over the cross-section. Materials with an apparent fine structure made from carbon black took up much more acid than materials with a more coarse apparent structure made from graphitized carbon. The same trend was evident from thermally accelerated fuel cell tests at 180 °C under constant load where degradation rates depended strongly on the choice of GDL material, especially on the cathode side. Acid was collected from the fuel cell exhaust at rates clearly correlated to the fuel cell degradation rates, but amounted to less than 6% of the total acid content in the cell even after significant degradation. Long-term durability of more than 5,500 h with a degradation rate of 12 µV h⁻¹ at 180 °C and 200 mA cm⁻² was demonstrated with the GDL that retained acid most efficiently.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors
Authors: Kannan, A. (Intern), Li, Q. (Intern), Cleemann, L. N. (Intern), Jensen, J. O. (Intern)
Pages: 103-112
Publication date: 2018
Main Research Area: Technical/natural sciences
Adiabatic and Nonadiabatic Charge Transport in Li-S Batteries

The insulating nature of the redox end members in Li-S batteries, -S and Li2S, has the potential to limit the capacity and efficiency of this emerging energy storage system. Nevertheless, the mechanisms responsible for ionic and electronic transport in these materials remain a matter of debate. The present study clarifies these mechanisms – in both the adiabatic and nonadiabatic charge transfer regimes – by employing a combination of hybrid-functional-based and constrained density functional theory calculations. Charge transfer in Li2S is predicted to be adiabatic, and thus is well described by conventional DFT methodologies. In sulfur, however, transitions between S8 rings are nonadiabatic. In this case, conventional DFT overestimates charge transfer rates by up to 2 orders of magnitude. Delocalized holes, and to a lesser extent, localized electron polarons, are predicted to be the most mobile electronic charge carriers in -S; in Li2S hole polarons dominate. Although all carriers exhibit extremely low equilibrium concentrations, and thus yield negligible contributions to the conductivity, their mobilities are sufficient to enable the sulfur loading targets necessary for high energy densities. Our results highlight the value of methods capable of capturing nonadiabaticity, such as constrained DFT. These techniques are especially important for molecular crystals such as -S, where longer-range charge transfer events are expected. Combining the present computational results with prior experimental studies, we conclude that low equilibrium carrier concentrations are responsible for sluggish charge transport in -S and Li2S. Thus, a potential strategy for improving the performance of Li-S batteries is to increase the concentrations of holes in these redox end members.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, University of Michigan
Authors: Park, H. (Ekstern), Kumar, N. (Ekstern), Melander, M. (Intern), Vegge, T. (Intern), García Lastra, J. M. (Intern), Siegel, D. J. (Intern)
Pages: 915-928
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information
Journal: Chemistry of Materials
Volume: 30
Issue number: 3
ISSN (Print): 0897-4756
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): SNIP 1.896 SJR 4.675 CiteScore 9.74
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 8.89 SJR 4.136 SNIP 1.883
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 3.958 SNIP 2.061 CiteScore 9.38
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 3.595 SNIP 2.222 CiteScore 8.89
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 3.666 SNIP 2.267 CiteScore 8.94
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 4.181 SNIP 2.247 CiteScore 8.1
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 3.488 SNIP 2.118 CiteScore 7.38
Amorphous saturated Cerium-Tungsten-Titanium oxide nanofibers catalysts for NOx selective catalytic reaction

Herein for the first time, Ce$_{0.184}$W$_{0.07}$Ti$_{0.748}$O$_{2-\delta}$ nanofibers are prepared by electrospinning to serve as catalyst in the selective catalytic reduction (SCR) process. The addition of cerium is proven to inhibit crystallization of TiO$_2$, yielding an amorphous TiO$_x$-based solid solution stable up to 500 °C in air, with supersaturated substitutional Ce. However, at higher temperatures, anatase phase (titanium oxide) is then observed along with fluorite (cerium oxide). Tungsten is instead demonstrated to promote the reduction of the Ce$^{4+}$ to Ce$^{3+}$ with formation of oxygen vacancies ($\delta$). Catalytic experiments at the best working conditions (dry and in absence of SO$_2$) are performed to characterize the intrinsic catalytic behavior of the new catalysts. At temperature lower than 300 °C, superior NOx conversion properties of the amorphous TiO$_x$ nanofibers over the crystallized TiO$_2$ (anatase) nanofibers are observed and attributed to higher specific surface area (SSA), larger amount of oxygen vacancies, and higher amount of Ce$^{3+}$ over the Ce$^{4+}$. Comparison with literature data for ceria-tungsten-based nanoparticles also points out higher catalytic performances for the developed nanofibers at the lowest temperatures (< 300°C). This is mainly attributed to the unique nanofibrous morphology and to the doping approach. Stability of the amorphous Ce-W-TiO$_x$ nanofibers over time (120 h) and over a number of cycles (5) is demonstrated. Yet, superior catalytic performances of the developed catalysts in a wide range of temperatures (200-500 °C) over state-of-the-art material V-W-titania nanoparticles and nanofibers are also proven.

General information

State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Imaging and Structural Analysis, Mixed Conductors, Silpakorn University, Technical University of Denmark
Authors: Dankeaw, A. (Intern), Gualandris, F. (Intern), Silva, R. H. (Ekstern), Norrman, K. (Intern), Gudik-Sørensen, M. (Intern), Kammer Hansen, K. (Intern), Ksapabutr, B. (Ekstern), Esposito, V. (Intern), Marani, D. (Intern)
Pages: 9501-9509
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information
Journal: New Journal of Chemistry
Volume: 42
In this work we study the degradation of roll-coated flexible inverted organic solar cells in different atmospheres. We demonstrate that impedance spectroscopy is a powerful tool for elucidating degradation mechanisms; it is used here to distinguish the different degradation mechanisms due to water and oxygen. Identical cells were exposed to different accelerated degradation environments using water only, oxygen only, and both water and oxygen simultaneously, all of...
them enhanced with UV light. The photocurrent is dramatically reduced in the oxygen-degraded samples. Impedance measurements indicate that this phenomenon is attributed to defects introduced by absorption of oxygen, which results in an increase of the acceptor impurity (NA) at the cathode interface obtained from a Mott-Schottky analysis. Simultaneously, at the anode interface where PEDOT:PSS is not shielded by the substrate, the nature of degradation differs for the water and oxygen degraded samples. While oxygen + UV light decreases the conductivity of the PEDOT:PSS layer, water + UV light changes the PEDOT:PSS work function inducing a depletion region at the anode.
A Novel Algorithm for Lifetime Extrapolation, Prediction, and Estimation of Emerging PV Technologies

Accurate determination of the lifetime of novel hybrid and organic solar cells is often rather challenging due to the very dynamic behavior of such cells over time and ageing curves with shapes of varying nature. Therefore, in order to accurately and reproducibly determine the lifetime of photovoltaic devices with such a behavior, a novel elaboration algorithm is developed, which enables automatic smoothing, filtering, and extrapolation of the real lifetime data and reproducible determination of the lifetime parameters defined in the International Summit on OPV Stability guiding standards. The algorithm is also capable of predicting the lifetime of devices, not tested until the end of sample life, given that there is sufficient number of measured data points to perform reliable extrapolation of ageing curves (to a limited time frame). The algorithm is discussed in detail and a range of examples for different lifetime data are presented.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Organic Energy Materials, University of Padova
Authors: Rizzo, A. (Ekstern), Cester, A. (Ekstern), Madsen, M. V. (Intern), Krebs, F. C. (Intern), Gevorgyan, S. A. (Intern)
Number of pages: 9
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information
Journal: Small Methods
Volume: 2
Issue number: 1
Article number: 1700285
ISSN (Print): 2366-9608
Original language: English
DOIs: 10.1002/smtd.201700285
Source: FindIt
Source-ID: 2393861595
Publication: Research - peer-review › Journal article – Annual report year: 2018

A novel catalyst layer structure based surface-patterned Nafion® membrane for high-performance direct methanol fuel cell
Conventional catalyst layer with a smooth surface exists the larger area of "catalytic dead zone" and reduces the utilization of catalyst. Based on this, a novel catalyst layer structure based surface-patterned Nafion® membrane was designed to achieve more efficient electrochemical reaction in this work. Surface-patterned Nafion® membranes were prepared by hot pressing with different pressures, and their swelling degrees reduced obviously with the increase of pressure, but proton conductivities of the membranes were almost unchanged. Pre-swelling and direct-spraying deposition methods were used to prepare the novel catalyst layer, and the effect of pressure on the performance of MEA was investigated. The results suggested that the peak power density of DMFC with optimal novel catalyst layer structure increased by 28.84%, the charge transfer resistances of anode and cathode reduced by 28.8% and 26.5% respectively, compared with the
conventional catalyst layer. Performance improvement is attributed to the fact that the novel catalyst layer structure optimizes the electrolyte membrane/catalyst layer and gas diffusion layer/catalyst layer interfacial structure, which increases the electrochemical reaction region and reaction sites. The novel catalyst layer with a three-dimensional curved surface structure enlarges the “three-phase boundaries (TPB)” and electrochemical active surface area (ECSA) of membrane electrode assembly (MEA). Therefore, this work provides an effective solution to achieve the high performance of DMFC by optimizing the internal interface structure of electrode, which is helpful to the future development of DMFC.

**General information**

State: Published  
Organisations: Department of Energy Conversion and Storage, Proton conductors, University of Science and Technology Beijing, University of Science and Technology of China  
Authors: Chen, M. (Ekstern), Wang, M. (Ekstern), Ding, X. (Ekstern), Li, Q. (Intern), Wang, X. (Ekstern)  
Pages: 201-208  
Publication date: 2018

**Main Research Area:** Technical/natural sciences

**Publication information**  
Journal: Electrochimica Acta  
Volume: 263  
ISSN (Print): 0013-4686  
Ratings:  
BFI (2018): BFI-level 2  
Web of Science (2018): Indexed yes  
BFI (2017): BFI-level 2  
Web of Science (2017): Indexed yes  
Scopus rating (2017): CiteScore 5.01 SJR 1.439 SNIP 1.101  
Web of Science (2017): Indexed yes  
BFI (2016): BFI-level 2  
Web of Science (2016): Indexed yes  
Scopus rating (2016): CiteScore 4.74 SJR 1.355 SNIP 1.177  
Web of Science (2016): Indexed yes  
BFI (2015): BFI-level 2  
Scopus rating (2015): SJR 1.321 SNIP 1.324 CiteScore 4.86  
Web of Science (2015): Indexed yes  
BFI (2014): BFI-level 2  
Scopus rating (2014): SJR 1.378 SNIP 1.456 CiteScore 4.59  
Web of Science (2014): Indexed yes  
BFI (2013): BFI-level 1  
Scopus rating (2013): SJR 1.427 SNIP 1.587 CiteScore 4.44  
ISI indexed (2013): ISI indexed yes  
Web of Science (2013): Indexed yes  
BFI (2012): BFI-level 1  
Scopus rating (2012): SJR 1.644 SNIP 1.574 CiteScore 3.99  
ISI indexed (2012): ISI indexed yes  
Web of Science (2012): Indexed yes  
BFI (2011): BFI-level 1  
Scopus rating (2011): SJR 1.615 SNIP 1.788 CiteScore 4.15  
ISI indexed (2011): ISI indexed yes  
Web of Science (2011): Indexed yes  
BFI (2010): BFI-level 1  
Scopus rating (2010): SJR 1.685 SNIP 1.715  
Web of Science (2010): Indexed yes  
BFI (2009): BFI-level 1  
Scopus rating (2009): SJR 1.523 SNIP 1.615  
BFI (2008): BFI-level 1  
Scopus rating (2008): SJR 1.524 SNIP 1.458  
Web of Science (2008): Indexed yes  
Scopus rating (2007): SJR 1.551 SNIP 1.568  
Web of Science (2007): Indexed yes
Assessment of potential biomass energy production in China towards 2030 and 2050
The objective of this paper is to provide a more detailed picture of potential biomass energy production in the Chinese energy system towards 2030 and 2050. Biomass for bioenergy feedstocks comes from five sources, which are agricultural crop residues, forest residues and industrial wood waste, energy crops and woody crops, animal manure, and municipal solid waste. The potential biomass production is predicted based on the resource availability. In the process of identifying biomass resources production, assumptions are made regarding arable land, marginal land, crops yields, forest growth rate, and meat consumption and waste production. Four scenarios were designed to describe the potential biomass energy production to elaborate the role of biomass energy in the Chinese energy system in 2030. The assessment shows that under certain restrictions on land availability, the maximum potential biomass energy productions are estimated to be 18,833 and 24,901 PJ in 2030 and 2050.

General information
State: Published
Organisations: Department of Energy Conversion and Storage
Authors: Zhao, G. (Intern)
Pages: 47-66
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information
Journal: International Journal of Sustainable Energy
Volume: 37
Issue number: 1
ISSN (Print): 1478-6451
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 1.17 SJR 0.471 SNIP 0.531
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 0.92 SJR 0.414 SNIP 0.719
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.346 SNIP 0.509 CiteScore 0.63
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.351 SNIP 0.568 CiteScore 0.73
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.337 SNIP 0.727 CiteScore 0.88
ISI indexed (2013): ISI indexed no
BFI (2012): BFI-level 1
A three dimensional multiphysics model of a solid oxide electrochemical cell: A tool for understanding degradation

Mitigating degradation is essential for extending the lifetime of solid oxide electrochemical cells (SOCs). The conditions leading to degradation, e.g. overpotentials, gas partial pressures, thermal gradients are hard, if not impossible, to retrieve experimentally. Thus, to deconvolute the response from cell testing, modeling can be applied to understand the degradation phenomena in greater detail. Modeling of SOCs is well developed. For computational efficiency, the electrodes are often represented with a mathematical abstraction of zero thickness layer. In this work, further attention is given to the local conditions in the through-thickness of the electrodes, by rigidly integrating classical electrochemistry into a three dimensional multiphysics model of an SOC. Hereby, local conditions (e.g. overpotential) vary through the electrode, and with the coupling to the different transport phenomena occurring (mass, current, momentum and species), this becomes available in three dimensions, throughout a cell. To investigate the validity of the model, a high number of experiments are conducted at different operating conditions, i.e. in both fuel cell and electrolysis mode of operation with H₂ / H₂O as feedstock varying parameters such as temperature, gas flows and gas compositions.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Applied Electrochemistry, Lund University
Authors: Navasa, M. (Intern), Graves, C. (Intern), Skafte, T. L. (Intern), Sundén, B. (Ekstern), Frandsen, H. L. (Intern)
Number of pages: 19
Pages: 11913-11931
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information
Volume: 43
Issue number: 27
ISSN (Print): 0360-3199
Ratings:

BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 4.1 SJR 1.116 SNIP 1.267
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.74 SJR 1.145 SNIP 1.315
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.27 SNIP 1.314 CiteScore 3.46
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.207 SNIP 1.484 CiteScore 3.54
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.265 SNIP 1.449 CiteScore 3.38
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.499 SNIP 1.708 CiteScore 3.96
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.443 SNIP 1.828 CiteScore 4.42
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.579 SNIP 1.854
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.32 SNIP 1.87
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.389 SNIP 2.073
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.266 SNIP 2.197
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.061 SNIP 2.202
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.116 SNIP 1.825
Scopus rating (2004): SJR 1.232 SNIP 1.626
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 0.996 SNIP 1.289
Scopus rating (2002): SJR 0.748 SNIP 1.156
Scopus rating (2001): SJR 0.488 SNIP 1.197
Scopus rating (2000): SJR 0.384 SNIP 0.83
Scopus rating (1999): SJR 0.376 SNIP 0.882

Original language: English

Solid oxide electrochemical cells, Transport phenomena, Degradation, Potential profiles, Modeling

DOIs:

10.1016/j.ijhydene.2018.04.164
Source: PublicationPreSubmission
Source-ID: 148652668
A topology optimized switchable permanent magnet system

The design of a magnetic field source that can switch from a high field to a low field configuration by rotation by 90° of a set of iron pieces is investigated using topology optimization. A Halbach cylinder is considered as the magnetic field source and iron inserts are placed in the air gap of the Halbach cylinder. The ideal shape of these iron inserts is determined as a function of the field generated by the Halbach cylinder and as a function of the size of the iron segments. The topology optimized structures are parabolic shaped pieces and have a difference in flux density between the high and low positions that is on average 1.29 times higher than optimized regular pole pieces. The maximum increase is a factor of 2.08 times higher than the regular pole pieces.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Authors: Bjørk, R. (Intern), Insinga, A. R. (Intern)
Pages: 106-113
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication Information
Journal: Journal of Magnetism and Magnetic Materials
Volume: 465
ISSN (Print): 0304-8853
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SJR 0.786 SNIP 1.349 CiteScore 2.97
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.41 SJR 0.699 SNIP 1.181
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.73 SNIP 1.296 CiteScore 2.33
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.815 SNIP 1.423 CiteScore 2.07
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.801 SNIP 1.385 CiteScore 2.03
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.928 SNIP 1.294 CiteScore 1.95
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.07 SNIP 1.275 CiteScore 1.84
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.936 SNIP 0.987
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.844 SNIP 0.908
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Carbon Deposition Diagnostics for Reliability and State-of-Health Assessment of SOFC

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry
Authors: Ploner, A. (Intern), Hagen, A. (Intern), Hauch, A. (Intern)
Number of pages: 1
Publication date: 2018
Conference: 233rd ECS Meeting, Seattle, United States, 13/05/2018 - 13/05/2018
Main Research Area: Technical/natural sciences

Publication information
Journal: Electrochemical Society. Meeting Abstracts (Online)
Volume: MA2018-01
Article number: 1280
ISSN (Print): 2151-2043
Original language: English
Links: http://ma.ecsdl.org.proxy.findit.dtu.dk/content/MA2018-01/20/1280
Source: FindIt
Source-ID: 2304159427
Publication: Research - peer-review › Journal article – Annual report year: 2018

Operation of Solid Oxide Fuel Cells (SOFCs) with carbon-based fuels is a major advantage of this specific fuel cell technology. Yet, the use of carbon-containing fuels can lead to deactivation of the cell if carbon deposition occurs. Therefore, this study simulates failure on a Ni-YSZ-supported cell under steam reforming conditions by stopping the steam supply and investigates the cell voltage and temperature responses due to this fault. Simultaneously, time-dependent electrochemical impedance spectroscopy (EIS) monitoring during cell operation was performed which could be correlated to two processes, one mainly originating from support layer and another from the active anode layer of the cell in a Ni-YSZ supported cell. Monitoring via EIS may therefore be used to allow recognition of carbon deposition in due course and give the opportunity to counteract before detrimental failure occurs.
Catalyst Degradation Under Potential Cycling as an Accelerated Stress Test for PBI-Based High-Temperature PEM Fuel Cells - Effect of Humidification

In the present work, high-temperature polymer electrolyte membrane fuel cells were subjected to accelerated stress tests of 30,000 potential cycles between 0.6 and 1.0 V at 160 °C (133 h cycling time). The effect that humidity has on the catalyst durability was studied by testing either with or without humidification of the nitrogen that was used as cathode gas during cycling segments. Pronounced degradation was seen from the polarization curves in both cases, though permanent only in the humidified case. In the unhumidified case, the performance loss was more or less recoverable following 24 h of operation at 200 mA cm⁻². A difference in degradation behavior was verified with electron microscopy, X-ray diffraction, and electrochemical impedance spectroscopy. The strong effect of humidification is explained by drying of the phosphoric acid that is in the catalyst layer(s) versus maintaining humidification of this region. Catalyst degradation due to platinum dissolution, transport of its ions, and eventual recrystallization is reduced when this portion of the acid dries out. Consequently, catalyst particles are only mildly affected by the potential cycling in the unhumidified case.
Catalyst evaluation for oxygen reduction reaction in concentrated phosphoric acid at elevated temperatures

Phosphoric acid is the common electrolyte for high-temperature polymer electrolyte fuel cells (HT-PEMFCs) that have advantages such as enhanced CO tolerance and simplified heat and water management. The currently used rotating disk electrode technique is limited to tests in dilute solutions at low temperatures and hence is not suitable for catalyst evaluation for HT-PEMFCs. In this study, we have designed and constructed a half-cell setup to measure the intrinsic activities of catalysts towards the oxygen reduction reaction (ORR) in conditions close to HT-PEMFC cathodes. By optimization of the hydrophobic characteristics of electrodes and the catalyst layer thickness, ORR activities of typical Pt/C catalysts are successfully measured in concentrated phosphoric acid at temperatures above 100 °C. In terms of mass-specific activities, the catalyst exhibits about two times higher activity in the half-cell electrode than that observed in fuel cells, indicating the feasibility of the technique as well as the potential for further improvement of fuel cell electrode performance.
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Power Sources
Volume: 375
ISSN (Print): 0378-7753
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 7 SJR 2.202 SNIP 1.536
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 6.22 SJR 1.944 SNIP 1.5
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.9 SNIP 1.667 CiteScore 6.34
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.964 SNIP 2.042 CiteScore 6.3
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.975 SNIP 2.137 CiteScore 5.63
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.282 SNIP 2.006 CiteScore 5.04
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.227 SNIP 2.172 CiteScore 5.13
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 2.294 SNIP 1.972
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 2.105 SNIP 1.785
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.96 SNIP 1.713
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.587 SNIP 1.488
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.802 SNIP 2.223
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.656 SNIP 1.809
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.85 SNIP 1.805
Scopus rating (2003): SJR 1.66 SNIP 1.57
Scopus rating (2002): SJR 2.385 SNIP 1.409
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 1.146 SNIP 1.506
Scopus rating (2000): SJR 0.649 SNIP 0.949
Changing the Usual Interpretation of the Structure and Ground State of Cu²⁺-Layered Perovskites

Intense research on hybrid organic-inorganic layered copper perovskites are currently being carried out. Many interesting properties of these materials rest on the strong correlation between electronic structure and local geometry. As up to now no reliable information on the pressure dependence of Cu²⁺-X- distances (X = Cl, F) has been reported, we have derived them from first-principles calculations on several representative hybrid and inorganic Cu²⁺ layered compounds. As a salient feature, we find that in all cases the out-of-plane Cu²⁺-X- distance is nearly insensitive to pressure, contrary to what is found for the short and long in-plane distances. These results thus disprove the widely assumed idea that the local structure arises from a Jahn-Teller effect involving a principal axis in the layer plane. By contrast, the present work demonstrates that the ground state and the local geometry are governed by two main factors. On one hand, the axial internal electric field due to the rest of lattice ions, which favors placing the hole of the CuX₆⁻ unit in the 3z²-r² level. On the other hand, the existence of an additional orthorhombic instability in the layer plane that nevertheless preserves the dominant 3z²-r² character, in agreement with experimental data of pure and doped Cu²⁺ layered compounds. This instability is favored in pure compounds by a cooperative mechanism that is also discussed. The present calculations on these systems under pressure show that a slightly elongated CuX₆⁻ unit can also have the hole in the axial 3z²-r² level, an unexpected situation that can only be explained with the introduction of the often ignored internal electric field.

General information

State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, Universidad de Cantabria
Authors: Aramburu, J. A. (Ekstern), García-Fernández, P. (Ekstern), Mathiesen, N. R. (Intern), García-Lastra, J. M. (Intern), Moreno, M. (Ekstern)
Pages: 5071-5082
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Physical Chemistry C
Volume: 122
Issue number: 9
ISSN (Print): 1932-7447
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 4.58 SJR 2.135 SNIP 1.147
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.48 SJR 1.964 SNIP 1.195
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.886 SNIP 1.26 CiteScore 4.68
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.032 SNIP 1.447 CiteScore 5.08
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 2.143 SNIP 1.445 CiteScore 5.14
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Chemically controlled interfacial nanoparticle assembly into nanoporous gold films for electrochemical applications

Nanoporous gold (NPG) is an effective material for electrocatalysis and can be made via a dealloy method such as etching of silver–gold alloys. Dealloyed NPG may contain residual silver that affects its catalytic performance. Herein, a different approach has been reported for the formation of NPG at the liquid/air interface starting from gold nanoparticles (AuNPs) in an aqueous solution, providing silver-free gold films. Chloroauric acid is reduced to AuNP building blocks by 2-(N-morpholino)ethanesulfonic acid, which also acts as a protecting agent and pH buffer. By adding potassium chloride before AuNP synthesis and hydrochloric acid to the resultant AuNP solutions, we can reproducibly obtain continuous gold networks. The sintered AuNPs produced by this method result in chemically synthesized nanoporous gold films (cNPGFs) that resemble dealloyed NPG in terms of morphology and porosity; additionally, they can be controlled by varying the temperature, chloride concentration, ionic strength, and protonation of the buffer. cNPGF formation is attributed to the destabilization of AuNPs at the air–liquid interface. The developed method generates electrochemically stable cNPGFs up to 20 cm² in size with an average thickness of 500 ± 200 nm, areal density of 50–150 μg cm⁻², and porosity as high as 85%. Importantly, cNPGFs can effectively catalyze both CO₂ reduction and CO oxidation electrochemically. Thus, the developed synthetic method offers large-scale production of pure bottom-up NPGFs for multifarious electrocatalytic applications.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Department of Chemistry, NanoChemistry, Organic Chemistry, Department of Biotechnology and Biomedicine, Technical University of Denmark
Authors: Christiansen, M. U. -. (Ekstern), Seselj, N. (Intern), Engelbrekt, C. (Intern), Wagner, M. (Intern), Stappen, F. N. (Ekstern), Zhang, J. (Intern)
Pages: 556-564
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Materials Chemistry A
Citrate- and glycerol triesters as novel dual-functional dispersants and plasticisers for ceramic processing

Short chained triesters of glycerol and citric acid were systematically investigated as novel dual-functional dispersants and plasticisers for use in ceramic processing. Additional systematic studies on a series of diesters having structural similarities with the citrate and glycerol triesters were performed to further assess the significance of specific functional groups for the stabilisation of suspensions.

The overall purpose of this work consists in simplifying the formulation for ceramic processing slurries while at the same time limiting the environmental impact and toxicity. The use of multifunctional additives reduces the risk of unwanted interactions between different components. Additionally, the possible use of one additive in more than one role opens the opportunity for an overall reduction in the number and amount of chemicals and therefore reduction of costs and risks.

For the citrate ester candidates, different alkoxy groups were tested as well as the acetylation on the hydroxyl group. The glycerol esters differed by the length of the carboxylic chain.

Especially triethyl and tributyl citrate are proposed as promising dual-functional additives for ceramic processing. Specifically, for triethyl citrate the dual-function was finally demonstrated by producing a dense piece of 8YSZ through tape casting and subsequent sintering.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Imaging and Structural Analysis
Authors: Foghmoes, S. (Intern), Klemensø, T. (Intern), Brodersen, K. (Intern), Bentzen, J. J. (Intern), Della Negra, M. (Intern)
Number of pages: 8
Pages: 9132-9139
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information
Journal: Ceramics International
Volume: 44
Issue number: 8
ISSN (Print): 0272-8842
Ratings:
BFI (2018): BFI-level 1
Classical statistical methodology for accelerated testing of Solid Oxide Fuel Cells

Solid Oxide Fuel Cell (SOFC) lifetime prognosis is a substantial challenge for market introduction. This paper illustrates an accelerated testing approach based on an extensive quantity of experimental degradation data and suggests derivable degradation quantities for SOFC with focus on a large number of tests. The semi-empirical degradation models are based on the underlying physical degradation phenomena in the cell and are used for projection of temperature and steam impact on SOFC aging. Degradation tests performed at seven different temperatures and four different p(H2O) in the fuel gas are used for evaluation. The key contribution of this study is parameterization of the aging model by experimental data.
while physical simulations in literature usually lack such robust empirical foundation.

**General information**

State: Published  
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry  
Authors: Ploner, A. (Intern), Hagen, A. (Intern), Hauch, A. (Intern)  
Pages: 379-385  
Publication date: 2018  
Main Research Area: Technical/natural sciences

**Publication information**

Journal: Journal of Power Sources  
Volume: 395  
ISSN (Print): 0378-7753  
Ratings:

- BFI (2018): BFI-level 1
- Web of Science (2018): Indexed yes
- BFI (2017): BFI-level 1
  - Scopus rating (2017): CiteScore 7 SJR 2.202 SNIP 1.536
  - Web of Science (2017): Indexed yes
- BFI (2016): BFI-level 1
  - Scopus rating (2016): CiteScore 6.22 SJR 1.944 SNIP 1.5
  - Web of Science (2016): Indexed yes
- BFI (2015): BFI-level 1
  - Scopus rating (2015): SJR 1.9 SNIP 1.667 CiteScore 6.34
  - Web of Science (2015): Indexed yes
- BFI (2014): BFI-level 1
  - Scopus rating (2014): SJR 1.964 SNIP 2.042 CiteScore 6.3
  - Web of Science (2014): Indexed yes
- BFI (2013): BFI-level 1
  - Scopus rating (2013): SJR 1.975 SNIP 2.137 CiteScore 5.63
  - ISI indexed (2013): ISI indexed yes
  - Web of Science (2013): Indexed yes
- BFI (2012): BFI-level 1
  - Scopus rating (2012): SJR 2.282 SNIP 2.006 CiteScore 5.04
  - ISI indexed (2012): ISI indexed yes
  - Web of Science (2012): Indexed yes
- BFI (2011): BFI-level 1
  - Scopus rating (2011): SJR 2.227 SNIP 2.172 CiteScore 5.13
  - ISI indexed (2011): ISI indexed yes
  - Web of Science (2011): Indexed yes
- BFI (2010): BFI-level 1
  - Scopus rating (2010): SJR 2.294 SNIP 1.972
  - Web of Science (2010): Indexed yes
- BFI (2009): BFI-level 1
  - Scopus rating (2009): SJR 2.105 SNIP 1.785
  - Web of Science (2009): Indexed yes
- BFI (2008): BFI-level 2
  - Scopus rating (2008): SJR 1.96 SNIP 1.713
  - Web of Science (2008): Indexed yes
- Scopus rating (2007): SJR 1.587 SNIP 1.488
  - Web of Science (2007): Indexed yes
- Scopus rating (2006): SJR 1.802 SNIP 2.223
  - Web of Science (2006): Indexed yes
- Scopus rating (2005): SJR 1.656 SNIP 1.809
  - Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.85 SNIP 1.805
Scopus rating (2003): SJR 1.66 SNIP 1.57
Scopus rating (2002): SJR 2.385 SNIP 1.409
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 1.146 SNIP 1.506
Scopus rating (2000): SJR 0.649 SNIP 0.949
Scopus rating (1999): SJR 0.814 SNIP 0.988
Original language: English
Solid oxide fuel cell, Accelerated testing, Lifetime prediction, Aging model
DOIs:
10.1016/j.jpowsour.2018.05.034
Source: FindIt
Source-ID: 2435341540
Publication: Research - peer-review › Journal article – Annual report year: 2018

clean energy materials innovation challenge

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, Department of Physics, Theoretical Atomic-scale Physics, Center for Nanostructured Graphene, Harvard University
Authors: Vegge, T. (Intern), Thygesen, K. S. (Intern), Aspuru-Guzik, A. (Ekstern)
Pages: 81-88
Publication date: 2018

Host publication information
Title of host publication: Accelerating the clean energy revolution - perspectives on innovation challenges : DTU International Energy Report 2018
Publisher: Technical University of Denmark (DTU)
ISBN (Electronic): 978-87-93458-57-4
Chapter: 10
Main Research Area: Technical/natural sciences
Electronic versions:
Publication: Research - peer-review › Report chapter – Annual report year: 2018

Co-deposition of CuO and Mn$_{1.5}$Co$_{1.5}$O$_4$ powders on Crofer22APU by electrophoretic method: Structural, compositional modifications and corrosion properties
Co-deposition of CuO and Mn$_{1.5}$Co$_{1.5}$O$_4$ by single step electrophoretic deposition is used to produce ~15µm coatings on Crofer22APU steel, which find use as interconnect for high temperature solid oxide cells. Sintering of the green coatings in reducing and then oxidizing conditions led to formation of a mixed (Cu,Mn,Co)$_2$O$_4$ spinel. By the incorporation of Cu, the density of the coatings improved. Scanning and transmission electron microscopy observations, supplemented with energy dispersive spectroscopy, confirmed dissolution of Cu in the spinel phase. For the un-doped Mn$_{1.5}$Co$_{1.5}$O$_4$ both the tetragonal and cubic phases are detected at room temperature by X-ray diffractometry, whereas the addition of Cu seems to stabilize the cubic phase. Initial (~1000h) high temperature corrosion evaluation at 800°C in air showed promising properties of the mixed spinel coating.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Politecnico di Torino, AGH University of Science and Technology, University of Erlangen-Nuremberg
Authors: Molin, S. (Intern), Sabato, A. G. (Ekstern), Javed, H. (Ekstern), Cempura, G. (Ekstern), Boccaccini, A. R. (Ekstern), Smeacetto, F. (Ekstern)
Pages: 329-333
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information
Journal: Materials Letters
Volume: 218
ISSN (Print): 0167-577X
Ratings:
Combinatorial selection of a two-dimensional 3d-TM-tetracyanoquinodimethane (TM-TCNQ) monolayer as a high-activity nanocatalyst for CO oxidation
The CO oxidation reaction on single 3d-transition metal catalytic sites in experimentally realized tetracyanoquinodimethane (TM-TCNQ) monolayers (TM = Sc-Zn) is systematically investigated by means of first-principles calculations. Considering the stabilities, adsorption characteristics and thermodynamics of all the ten candidates (Sc-Zn), Sc-TCNQ is found to display the lowest activation energies and yield the highest catalytic activity for room temperature CO oxidation. Exploring the Langmuir-Hinshelwood (LH) and Eley-Rideal (ER) mechanisms, we find that the rate-limiting step of CO oxidation catalyzed by Sc-TCNQ (CO + O2* → OOCO*) can follow the LH mechanism with free energy barriers as low as 0.73 eV at 300 K. The second step of CO + O* → CO2 can occur with rather small energy barriers via either LH or ER mechanisms. The high activity of Sc-TCNQ can be attributed to its unique structural and electronic features by possessing high stability, optimum adsorption energies with adsorbates, and fast reaction kinetics. These results have significant implications for the synthesis of two-dimensional single atom catalysis for CO oxidation with low-cost and high activity at low temperature.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, Huaiyin Normal University
Authors: Deng, Q. (Intern), Wu, T. (Intern), Chen, G. (Ekstern), Hansen, H. A. (Intern), Vegge, T. (Intern)
Pages: 5173-5179
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information
Journal: Physical Chemistry Chemical Physics
Volume: 20
Issue number: 7
ISSN (Print): 1463-9076
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 4.04 SJR 1.686 SNIP 1.089
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.06 SJR 1.685 SNIP 1.113
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.725 SNIP 1.205 CiteScore 4.45
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.771 SNIP 1.239 CiteScore 4.29
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.72 SNIP 1.207 CiteScore 4.05
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.921 SNIP 1.177 CiteScore 3.67
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.707 SNIP 1.19 CiteScore 3.6
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.817 SNIP 1.199
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.147 SNIP 1.364
Combined DFT and DEMS investigation of the effect of dopants in secondary zinc-air batteries

Zinc–air batteries offer the potential of low-cost energy storage with high specific energy, but at present secondary Zn–air batteries suffer from poor cyclability. To develop economically viable secondary Zn–air batteries, several properties need to be improved: choking of the cathode, catalyzing the oxygen evolution and reduction reactions, limiting dendrite formation and suppressing the hydrogen evolution reaction (HER). Understanding and alleviating HER at the negative electrode in a secondary Zn–air battery is a substantial challenge, for which it is necessary to combine computational and experimental research. Here, we combine differential electrochemical mass spectrometry (DEMS) and density functional theory (DFT) calculations to investigate the fundamental role and stability when cycling in the presence of selected beneficial additives, that is, In and Bi, and Ag as a potentially unfavorable additive. We show that both In and Bi have the desired property for a secondary battery, that is, upon recharging they will remain on the surface, thereby retaining the beneficial effects on Zn dissolution and suppression of HER. This is confirmed by DEMS, where it is observed that In reduces HER and Bi affects the discharge potential beneficially compared to a battery without additives. Using a simple procedure based on adsorption energies calculated with DFT, it is found that Ag suppresses OH adsorption, but, unlike In and Bi, it does not hinder HER. Finally, it is shown that mixing In and Bi is beneficial compared to the additives by themselves as it improves the electrochemical performance and cyclic stability of the secondary Zn–air battery.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials
Authors: Lysgaard, S. (Intern), Christensen, M. K. (Intern), Hansen, H. A. (Intern), García Lastra, J. M. (Intern), Norby, P. (Intern), Vegge, T. (Intern)
Pages: 1933-1941
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information
Journal: ChemSusChem (Print)
Volume: 11
Issue number: 12
ISSN (Print): 1864-5631
Ratings:
BFI (2018): BFI-level 2
Commercial alkaline earth boroaluminosilicate glasses for sealing solid oxide cell stacks. Part I: Development of glass-ceramic microstructure and thermomechanical properties

Sealing performance in solid oxide cell (SOC) stacks and the devitrification process of commercially available alkaline earth boroaluminosilicate glasses containing 48-61 mol% SiO₂, 18-28 mol% CaO, 1-7 mol% MgO, 7-10 mol% Al₂O₃, 1-11 mol% B₂O₃ plus minor amounts of Na₂O, K₂O, FeO, and TiO₂ were investigated and quantified through analysis of phase assemblages as function of heat treatments above the glass transition temperatures using the electron microprobe and powder X-ray diffraction. For two of these glasses devitrification behavior was compared to the devitrification behavior of similar glasses produced in the laboratory. Glasses were characterized after annealing in air at 800°C and 850°C for up to 6 weeks. Even though the glasses lie within a relatively narrow compositional range, sealing performance and the resulting microstructures differed significantly. Best thermomechanical properties was developed in one of the laboratory-produced glasses, MCAS, which may be applied in SOC-stacks by allowing for a slow solidification in the range 750-800°C followed by crystallization at or slightly above 800°C. The relatively high thermal expansion coefficient (CTE) from RT-800°C, 11 × 10⁻⁶ K⁻¹, which was developed over ~1000 hours at 800°C, depends mainly on the formation of cristobalite and quartz as well as the presence of a residual glass phase. The glass ceramic sealant appears relatively stable over time, except for a slow transition of cristobalite to quartz, and can possibly show self-healing behavior if later
brought close to 850°C. Devitrification led to increases of the thermal expansion coefficients in all other glasses tested, but did not reach levels interesting for SOC-stack sealing.

**General information**

**State:** Published  
**Organisations:** Department of Energy Conversion and Storage, Mixed Conductors, University of Copenhagen  
**Authors:** Agersted, K. (Ekstern), Balic-Zunic, T. (Ekstern)  
**Pages:** 255-266  
**Publication date:** 2018  
**Main Research Area:** Technical/natural sciences

**Publication information**

**Journal:** International Journal of Applied Ceramic Technology  
**Volume:** 15  
**Issue number:** 2  
**ISSN (Print):** 1546-542X  
**Ratings:**  
Web of Science (2018): Indexed yes  
Scopus rating (2017): CiteScore 1.21 SJR 0.378 SNIP 0.684  
Web of Science (2017): Indexed Yes  
Scopus rating (2016): CiteScore 1.08 SJR 0.381 SNIP 0.674  
Scopus rating (2015): SJR 0.426 SNIP 0.816 CiteScore 1.28  
Web of Science (2015): Indexed yes  
Scopus rating (2014): SJR 0.486 SNIP 0.976 CiteScore 1.45  
Scopus rating (2013): SJR 0.589 SNIP 1.029 CiteScore 1.33  
ISI indexed (2013): ISI indexed yes  
Web of Science (2013): Indexed yes  
Scopus rating (2012): SJR 0.577 SNIP 0.878 CiteScore 1.27  
ISI indexed (2012): ISI indexed yes  
Scopus rating (2011): SJR 0.62 SNIP 1.124 CiteScore 1.37  
ISI indexed (2011): ISI indexed yes  
Scopus rating (2010): SJR 0.705 SNIP 1.168  
Web of Science (2010): Indexed yes  
Scopus rating (2009): SJR 0.849 SNIP 1.13  
Scopus rating (2008): SJR 0.965 SNIP 1.394  
Scopus rating (2007): SJR 0.695 SNIP 1.249  
Scopus rating (2006): SJR 0.857 SNIP 1.978  
Scopus rating (2005): SJR 0.59 SNIP 1.66  
**Original language:** English  
**Borosilicate glass, Glass-ceramics, Microstructure, Solid oxide cell stack sealing**  
**DOIs:**  
10.1111/ijac.12829  
**Source:** FindIt  
**Source-ID:** 2393190618  
**Publication:** Research - peer-review › Journal article – Annual report year: 2018

**Commercial alkaline earth boroaluminosilicate glasses for sealing solid oxide cell stacks Part II: Characterization of devitrification and glass-ceramic phase assemblages**

The devitrification process and formation of crystalline phases from commercial alkaline earth boroaluminosilicate glasses containing 48-61 mol% SiO₂, 18-28 mol% CaO, 1-7 mol% MgO, 7-10 mol% Al₂O₃, 1-11 mol% B₂O₃ plus minor amounts of Na₂O, K₂O, FeO and TiO₂ were quantified through analysis of phase assemblages as function of heat treatments above the glass transition temperatures using the electron microprobe and powder X-ray diffraction. Treatments at 800 °C and 850 °C lasted up to 6 weeks.

Results indicate that devitrification was strongly activated through presence of heterogeneous nucleation, and that the growth mechanism gradually changed from three-dimensional growth at the onset of devitrification towards one-dimensional growth in later stages, when heterogeneous nucleation was absent or less dominating.

Most glasses developed entangled and fibrous microstructures with little or no residual glass phase, which are adequate for rigid sealants, and only one of the laboratory analogue glasses, MCAS, developed microstructures with both more equiaxed grains and a considerable amount of residual glass phase, which may be adequate for more compliant and self-healing sealants as often required in SOC-applications.
Even though the glasses lie within a relatively narrow compositional range, resulting phase assemblages differed significantly. Anorthite (plagioclase) developed as the main crystalline phase in all samples together with pyroxene (or pyroxenoide) and cristobalite. Calcium-magnesium-silicate pyroxene (diopside) was in a large part replaced by the calcium-silicate pyroxenoid (wollastonite) in the samples where the mol-proportion MgO:CaO was 1:5 or lower. In samples with a very low MgO proportion and consequently a high CaO proportion, calcium metaborate and calcium aluminum borosilicate (okayamalite) crystallized among the main phases and these glasses crystallized completely within the period of heat treatment. Although cristobalite is metastable at the annealing temperatures, both α and β forms were rapidly formed in most of the samples, likely due to kinetic reasons. The presence of the latter is explained by the stabilization effect of Al and B substitution for Si compensated by Ca stuffing in the structure. The stuffed cristobalite transformed with time to quartz (at 800 °C) or quartz plus tridymite (at 850 °C). Boron was incorporated in the first crystallizing phases, especially diopside, substituting for Al and Si, but the so established substitution partly disappeared with time during the heat treatment.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, University of Copenhagen
Authors: Agersted, K. (Ekstern), Balic-Zunic, T. (Ekstern)
Pages: 267-285
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information
Journal: International Journal of Applied Ceramic Technology
Volume: 15
Issue number: 2
ISSN (Print): 1546-542X
Ratings:
Web of Science (2018): Indexed yes
Scopus rating (2017): CiteScore 1.21 SJR 0.378 SNIP 0.684
Web of Science (2017): Indexed Yes
Scopus rating (2016): CiteScore 1.08 SJR 0.381 SNIP 0.674
Scopus rating (2015): SJR 0.426 SNIP 0.816 CiteScore 1.28
Web of Science (2015): Indexed yes
Scopus rating (2014): SJR 0.486 SNIP 0.976 CiteScore 1.45
Scopus rating (2013): SJR 0.589 SNIP 1.029 CiteScore 1.33
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Scopus rating (2012): SJR 0.577 SNIP 0.878 CiteScore 1.27
ISI indexed (2012): ISI indexed yes
Scopus rating (2011): SJR 0.62 SNIP 1.124 CiteScore 1.37
ISI indexed (2011): ISI indexed yes
Scopus rating (2010): SJR 0.705 SNIP 1.168
Web of Science (2010): Indexed yes
Scopus rating (2009): SJR 0.849 SNIP 1.13
Scopus rating (2008): SJR 0.965 SNIP 1.394
Scopus rating (2007): SJR 0.695 SNIP 1.249
Scopus rating (2006): SJR 0.857 SNIP 1.978
Scopus rating (2005): SJR 0.59 SNIP 1.66
Original language: English
DOIs:
10.1111/ijac.12834
Source: FindIt
Source-ID: 2393587869
Publication: Research - peer-review › Journal article – Annual report year: 2018

Communication—Perovskite Electrochemical System for Highly Selective NOx Reduction of Diesel Engine Exhaust
A perovskite electrochemical system was developed for selective NOx reduction of diesel engine exhaust. The system was composed of a La0.9Sr0.1CoO3±δ oxidation catalyst and a (La0.85Sr0.15)0.95MnO3±δ/Ce0.9Gd0.1O1.95 electrochemical cell with BaO nanoparticles. A selectivity of 25–35% was achieved with a NOx conversion of 65–75% in 1000 ppm NO with 8% O2 at 375°C. The superior performance of the system was suggested to be ascribed to the promotion in NO2 formation substantially activating the NOx trapping and reduction processes on the electrode.
Comparative DFT+U and HSE Study of the Oxygen Evolution Electrocatalysis on Perovskite Oxides

The most common method for incorporating strong electron correlations is either to apply the Hubbard U correction on top of standard density functional theory calculations (DFT) or to use hybrid functionals. In this study, we elucidate the sensitivity of the Hubbard U correction in the PBE+U functional and the amount of exact exchange, $\alpha$, in the hybrid HSE functional on the structural stability, catalytic activity and electronic conductivity of pure and doped perovskite oxides, $\text{ABO}_3$, ($A = \text{La, Ca, Sr and Ba}$, $B = \text{Cr, Mn, Fe, Co, Ni and Cu}$) for oxygen evolution electrocatalysis. We find a strong dependence of heat of formations and reaction overpotentials for a range of $U = 0, 3$ and $5$ eV and $\alpha = 0, 0.15, 0.25, 0.35$ values investigated in this study, which we attribute primarily to changes in the oxidation state of B cations. If the valence of B cations in the perovskite and reference oxide is the same, then the U- and $\alpha$ dependence is very small. On the other hand, if the valences are different then heat of formations can change by as much as 1 eV. As the oxidation state of a surface metal ion depends on adsorbed intermediate and nature of the element, similar differences in energies appear in the calculated reaction overpotentials for oxygen evolution. The large U and $\alpha$ dependence sets serious constraints on the use of DFT+U and HSE methods for assessing stabilities and catalytic activities of perovskite oxides. In addition, the large $\alpha$ dependence raises the question whether HSE calculations can improve sufficiently the accuracy of DFT+U results for multi-step electrochemical reactions to justify the excess computational cost. Although we have investigated only one particular class of catalysts and one electrochemical reaction, the results of this study can expectedly be generalized to other strongly correlated systems in which the oxidation state of the surface changes during reaction. The influence of U on the electronic conductivity is significant only in cases where it qualitatively changes the electronic structure, by e.g. opening the band-gap. From a combinatorial analysis on pure and doped oxides, we identify electronically conductive catalysts classified according to different electron conduction types: intrinsic conductivity ($\text{Fe}^{4+}$, $\text{Co}^{3+}$,(intermediate spin, IS) and $\text{Ni}^{3+}$), electron polaron hopping (along $\text{Mn}^{3+}$-$\text{O}$-$\text{Mn}^{4+}$ chains) and charge transport through holes in the valence band.
Comparison between La$_{0.6}$Sr$_{0.4}$CoO$_3$-d and LaNi$_{0.6}$Co$_{0.4}$O$_3$-d infiltrated oxygen electrodes for long-term durable solid oxide fuel cells

The degradation of infiltrated oxygen electrodes during long-term operation of solid oxide fuel cells (SOFCs) was studied. The infiltrated oxygen electrodes were prepared by infiltration of the electro-catalysts La$_{0.6}$Sr$_{0.4}$CoO$_3$-d (LSC) and LaNi$_{0.6}$Co$_{0.4}$O$_3$-d (LCN) into a porous yttria stabilized zirconia (YSZ) backbone that was pre-infiltrated with a gadolinium doped ceria (CGO) barrier layer. The performance of the infiltrated LSC and LCN electro-catalysts were compared for both symmetrical cells and full SOFCs. Galvanostatic long-term performance tests up to 1400 hours at 700°C and 0.5 A/cm$^2$ were conducted and the change of resistance was followed by electrochemical impedance spectroscopy under current load. The cell performance degradation profiles of the LSC and LCN infiltrated cells showed significant differences. The performance of the LSC infiltrated cell stabilized after 700 hours of operation and the LCN infiltrated cell degraded throughout the entire testing period. The difference between the intrinsic properties, i.e. its electrochemical activity, ionic conductivity,
and reactivity of LSC and LCN materials was hypothesized to be responsible for the observed difference in the degradation profile.

**General information**

State: Published
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry, Mixed Conductors
Authors: Ovtar, S. (Intern), Hauch, A. (Intern), Veltzé, S. (Intern), Chen, M. (Intern)
Pages: 293-304
Publication date: 2018
Main Research Area: Technical/natural sciences

**Publication information**

Journal: Electrochimica Acta
Volume: 266
ISSN (Print): 0013-4686
Ratings:

- BFI (2018): BFI-level 2
- Web of Science (2018): Indexed yes
- BFI (2017): BFI-level 2
- Scopus rating (2017): CiteScore 5.01 SJR 1.439 SNIP 1.101
- Web of Science (2017): Indexed yes
- BFI (2016): BFI-level 2
- Scopus rating (2016): CiteScore 4.74 SJR 1.355 SNIP 1.177
- Web of Science (2016): Indexed yes
- BFI (2015): BFI-level 2
- Scopus rating (2015): SJR 1.321 SNIP 1.324 CiteScore 4.86
- Web of Science (2015): Indexed yes
- BFI (2014): BFI-level 2
- Scopus rating (2014): SJR 1.378 SNIP 1.456 CiteScore 4.59
- Web of Science (2014): Indexed yes
- BFI (2013): BFI-level 1
- Scopus rating (2013): SJR 1.427 SNIP 1.587 CiteScore 4.44
- ISI indexed (2013): ISI indexed yes
- Web of Science (2013): Indexed yes
- BFI (2012): BFI-level 1
- Scopus rating (2012): SJR 1.644 SNIP 1.574 CiteScore 3.99
- ISI indexed (2012): ISI indexed yes
- Web of Science (2012): Indexed yes
- BFI (2011): BFI-level 1
- Scopus rating (2011): SJR 1.615 SNIP 1.788 CiteScore 4.15
- ISI indexed (2011): ISI indexed yes
- Web of Science (2011): Indexed yes
- BFI (2010): BFI-level 1
- Scopus rating (2010): SJR 1.685 SNIP 1.715
- Web of Science (2010): Indexed yes
- BFI (2009): BFI-level 1
- Scopus rating (2009): SJR 1.523 SNIP 1.615
- BFI (2008): BFI-level 1
- Scopus rating (2008): SJR 1.524 SNIP 1.458
- Web of Science (2008): Indexed yes
- Scopus rating (2007): SJR 1.551 SNIP 1.568
- Web of Science (2007): Indexed yes
- Scopus rating (2006): SJR 1.531 SNIP 1.726
- Web of Science (2006): Indexed yes
- Scopus rating (2005): SJR 1.484 SNIP 1.516
- Web of Science (2005): Indexed yes
Computational screening of doped αMnO2 catalysts for the oxygen evolution reaction

Minimizing energy and materials costs for driving the oxygen evolution reaction (OER) is paramount for the commercialization of water electrolysis cells and rechargeable metal-air batteries. Using density functional theory calculations, we analyze the structural stability, catalytic activity and electronic conductivity of pure and doped αMnO2 for the OER. As a model surface, we investigate the (110) and (100) facets, on which we identify three possible active sites: a coordination unsaturated, bridge and bulk site. We evaluate the performance of pure and Cr, Fe, Co, Ni, Cu, Zn, Cd, Mg, Al, Ga, In, Sc, Ru, Rh, Ir, Pd, Pt, Ti, Zr, Nb and Sn doped αMnO2. At each site and for each dopant, we impose the preferred valence by adding/subtracting electron donors (hydrogens) and electron acceptors (hydroxyls). From a subset of stable dopants, we identify Pd doped αMnO2 as the only catalyst that can outperform pristine αMnO2. We also discuss approaches to increase the electron conductivity as pure αMnO2 is a narrow band-gap material.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials
Authors: Tripkovic, V. (Intern), Hansen, H. A. (Intern), Vegge, T. (Intern)
Pages: 629-637
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information
Journal: ChemSusChem (Print)
Volume: 11
Issue number: 3
ISSN (Print): 1864-5631
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 6.86 SJR 2.538 SNIP 1.235
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 6.7 SJR 2.505 SNIP 1.311
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 2.53 SNIP 1.424 CiteScore 7.33
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.864 SNIP 1.663 CiteScore 7.97
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 2.561 SNIP 1.46 CiteScore 6.79
Efficient conversion of solar energy into electricity or fuels requires the identification of new semiconductors with optimal optical and electronic properties. We discuss the current and future role that computational screening is expected to play in this challenge. We discuss the identification of new computable descriptors characterising optimal materials performance, and we outline different search strategies in the materials screening. Finally, we describe some of the screening results obtained for perovskites, 2D materials, and for materials extracted from crystallographic databases.

**General information**

State: Published

**Organisations:** Department of Energy Conversion and Storage, Atomic scale modelling and materials, Department of Physics, Theoretical Atomic-scale Physics

**Authors:** Castelli, I. E. (Intern), Kuhar, K. (Intern), Pandey, M. (Intern), Jacobsen, K. W. (Intern)

**Pages:** 62-99

**Publication date:** 2018

**Host publication information**

**Title of host publication:** Advances in Photoelectrochemical Water Splitting: Theory, Experiment and Systems Analysis

**Publisher:** Royal Society of Chemistry

**ISBN (Print):** 978-1-78262-925-2

**ISBN (Electronic):** 978-1-78801-446-5, 978-1-78262-986-3

**Chapter:** 3

**Main Research Area:** Technical/natural sciences

**DOIs:** 10.1039/9781782629863-00062

**Publication:** Research - peer-review › Book chapter – Annual report year: 2018

**Contact of ZnSb thermoelectric material to metallic electrodes using S-Bond 400 solder alloy**

ZnSb is one of the promising low-cost p-type thermoelectric materials for constructing waste heat recovery devices operating in the medium temperature region (250 – 400 °C). To obtain high performance, these devices require stable and low resistance contacts between thermoelectric materials and metallic electrodes. In this paper, we investigate the joining of ZnSb to Ni and Ag electrodes using a commercial solder alloy S-Bond 400 and hot-pressing technique. Ti and Cr layers are also introduced as a diffusion barrier and microstructure at the interfaces is observed by scanning electron microscopy. We found that S-bond 400 solder reacts with Ag and Ni electrodes to form different alloys at the interfaces. Cr
layer was found to be broken after joining, resulting in a thicker reaction/diffusion layer at the interface, while Ti layer was preserved.

**General information**
State: Accepted/In press
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Electrofunctional materials
Authors: Malik, S. A. (Intern), Le, T. H. (Intern), Van Nong, N. (Intern)
Number of pages: 7
Publication date: 2018
Conference: 15th European Conference on Thermoelectrics (ECT2017), Padua, Italy, 25/09/2017 - 25/09/2017
Main Research Area: Technical/natural sciences

**Publication information**
Journal: Materials Today: Proceedings
ISSN (Print): 2214-7853
Ratings:
Scopus rating (2017): SNIP 0.837 SJR 0.314 CiteScore 0.94
Scopus rating (2016): CiteScore 0.43 SNIP 0.379 SJR 0.205
Scopus rating (2015): SNIP 0.364 SJR 0.463
Original language: English
Source: PublicationPreSubmission
Source-ID: 144763080
Publication: Research - peer-review › Conference article – Annual report year: 2018

**Continuous Hydrothermal Flow Synthesis of Gd-doped CeO₂ (GDC) Nanoparticles for Inkjet Printing of SOFC Electrolytes**
GdₐCe₁₋ₐO₂₋₅ (GDC) nanoparticles were synthesized using continuous hydrothermal flow synthesis. By varying the synthesis conditions, particle size and morphology could be tailored. Here, particle sizes between 6 to 40 nm with polyhedral or octahedral shape could be obtained. Gd₀.₂Ce₀.₈O₂₋₅ nanoparticles were further processed into inks for inkjet printing. Despite the small particle size/large surface area, inks with excellent printing behavior were formulated. For proof-of-concept, thin GDC layers were printed on a) green NiO-GDC substrates, and on b) pre-sintered NiO-YSZ substrates. While no dense layers could be obtained on the green NiO-GDC substrates, GDC nanoparticles printed on NiO-YSZ substrates formed a dense continuous layer after firing at 1300 °C.

**General information**
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Mixed Conductors, Applied Electrochemistry, Imperial College London
Authors: Xu, Y. (Intern), Farandos, N. M. (Ekstern), Rosa, M. (Intern), Zielke, P. (Intern), Esposito, V. (Intern), Hendriksen, P. V. (Intern), Jensen, S. H. (Intern), Li, T. (Ekstern), Kelsall, G. H. (Ekstern), Kiebach, W. (Intern)
Pages: 315-327
Publication date: 2018
Main Research Area: Technical/natural sciences

**Publication information**
Journal: International Journal of Applied Ceramic Technology
Volume: 15
Issue number: 2
ISSN (Print): 1546-542X
Ratings:
Web of Science (2018): Indexed yes
Scopus rating (2017): CiteScore 1.21 SJR 0.378 SNIP 0.684
Web of Science (2017): Indexed Yes
Scopus rating (2016): CiteScore 1.08 SJR 0.381 SNIP 0.674
Scopus rating (2015): SJR 0.426 SNIP 0.816 CiteScore 1.28
Web of Science (2015): Indexed yes
Scopus rating (2014): SJR 0.486 SNIP 0.976 CiteScore 1.45
Scopus rating (2013): SJR 0.589 SNIP 1.029 CiteScore 1.33
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Scopus rating (2012): SJR 0.577 SNIP 0.878 CiteScore 1.27
ISI indexed (2012): ISI indexed yes
Continuous Hydrothermal Flow Synthesis of LaCrO3 in Supercritical Water and Its Application in Dual-Phase Oxygen Transport Membranes

The continuous production of LaCrO3 particles (average edge size 639 nm, cube-shaped) by continuous hydrothermal flow synthesis using supercritical water is reported for the first time. By varying the reaction conditions, it was possible to suggest a reaction mechanism for the formation of this perovskite material. Moreover, dual-phase oxygen transport membranes were manufactured from the as-synthesized LaCrO3 particles and (ZrO2)0.89(Y2O3)0.01(Sc2O3)0.10 (10Sc1YSZ), and oxygen permeation fluxes up to 5 × 10–8 mol cm–2 s–1 were measured on a 1 mm thick membrane.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Quantitative Sustainability Assessment, Department of Management Engineering, Western Macedonia University of Applied Sciences
Authors: Chatzisideris, M. D. (Intern), Laurent, A. (Intern), Christoforidis, G. C. (Ekstern), Krebs, F. C. (Intern)
Pages: 425
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information
Journal: Applied Energy
Volume: 219
Cr- and Ti-Based Spinels as Materials for Anodic Catalyst Support in PEM Electrolysis Cells: Assessing Corrosion Stability and Support Role in Catalyst Activity of Corrosion Stable Ceramics

This work aims to determine the stability of Cr- and Ti-based spinels as catalyst supports for oxygen evolution reaction (OER) catalyst in PEM electrolyzers (PEMECs). Different compositions of MCr2O4 (M=Ni, NiFe, Zn, Mg) and MTi2O4 (Li, Mg, Mn) have been synthesized by solid state synthesis. Pure and doped Cr-based spinels exhibit low conductivities at the operating temperatures of PEMECs (1.5 V vs SHE). LiTi2O4 is completely oxidized upon cycling up to 2.0 V vs SHE. Mixtures of IrO2/oxide support deposited on glassy carbon were tested toward OER, which showed a 10% higher absolute current at 2.0 V vs SHE in the case of IrO2/Cu-MnCr2O4 compared with pure IrO2.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrochemical Materials and Interfaces, University of St Andrews
Authors: Fenini, F. (Intern), Hansen, K. K. (Intern), Savaniu, C. (Ekstern), Irvine, J. T. S. (Ekstern), Mogensen, M. B. (Intern)
Pages: 65-77
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information
Journal: E C S Transactions
Volume: 85
Issue number: 11
ISSN (Print): 1938-5862
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 0.44 SJR 0.225 SNIP 0.252
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 0.4 SJR 0.228 SNIP 0.253
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.211 SNIP 0.244 CiteScore 0.36
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.212 SNIP 0.234 CiteScore 0.36
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.192 SNIP 0.231 CiteScore 0.27
ISI indexed (2013): ISI indexed no
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.241 SNIP 0.26 CiteScore 0.29
ISI indexed (2012): ISI indexed no
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.261 SNIP 0.28 CiteScore 0.36
ISI indexed (2011): ISI indexed no
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.249 SNIP 0.251
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.242 SNIP 0.27
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.254 SNIP 0.255
Scopus rating (2007): SJR 0.213 SNIP 0.206
Scopus rating (2006): SJR 0.134 SNIP 0.073
Original language: English
DOIs:
10.1149/08511.0065ecst
Source: FindIt
Source-ID: 2434134952
**Cr- and Ti-Based Spinels As Materials for Anodic Catalyst Support in PEM Electrolysis Cells: Assessing Corrosion Stability and Support Role in Catalyst Activity of Corrosion Stable Ceramics**

**General information**
- **State:** Published
- **Organisations:** Department of Energy Conversion and Storage, University of St Andrews
- **Authors:** Fenini, F. (Intern), Kammer Hansen, K. (Intern), Savaniu, C. (Ekstern), Irvine, J. T. S. (Ekstern), Mogensen, M. B. (Intern)
- **Number of pages:** 1
- **Publication date:** 2018
- **Conference:** 233rd ECS Meeting, Seattle, United States, 13/05/2018 - 13/05/2018
- **Main Research Area:** Technical/natural sciences

**Publication information**
- **Journal:** Electrochemical Society. Meeting Abstracts (Online)
- **Volume:** MA2018-01
- **Article number:** 1661
- **ISSN (Print):** 2151-2043
- **Original language:** English
- **Links:** [http://ma.ecsd.org.proxy.findit.dtu.dk/content/MA2018-01/29/1661](http://ma.ecsd.org.proxy.findit.dtu.dk/content/MA2018-01/29/1661)
- **Source:** FindIt
- **Source-ID:** 2304160758

**Critical current density improvements in MgB2 superconducting bulk samples by K2CO3 additions**
MgB2 bulk samples with potassium carbonate doping were made by means of reaction of elemental Mg and B powders mixed with various amounts of K2CO3. The Tc of the superconducting phase as well as its a-axis parameter were decreased as a result of carbon doping. Potassium escaped the samples during reaction. The critical current density of MgB2 was improved both in self field and under applied magnetic field for T ≤ 30 K, with optimum results for 1 mol% K2CO3 addition. The normalized flux pinning force (f/b) shows that the flux pinning mechanism at low field is similar for all samples, following the predictions of the point pinning model. In contrast the behavior of f/b is significantly altered at reduced fields (b) larger than unity by K2CO3 additions, tending towards surface pinning. Besides providing carbon, another effect of K2CO3 may originate from the presence of a transient liquid phase that appears to improve the crystallinity and thus the critical current density at low field.

**General information**
- **State:** Published
- **Organisations:** Department of Energy Conversion and Storage, Electrofunctional materials
- **Authors:** Grivel, J. (Intern)
- **Pages:** 1-6
- **Publication date:** 2018
- **Main Research Area:** Technical/natural sciences

**Publication information**
- **Journal:** Physica C: Superconductivity and its Applications
- **Volume:** 550
- **ISSN (Print):** 0921-4534
- **Ratings:**
  - BFI (2018): BFI-level 1
  - Web of Science (2018): Indexed yes
  - BFI (2017): BFI-level 1
  - Scopus rating (2017): SNIP 0.858 SJR 0.492 CiteScore 1.28
  - Web of Science (2017): Indexed Yes
  - BFI (2016): BFI-level 1
  - Scopus rating (2016): CiteScore 1.14 SJR 0.467 SNIP 0.822
  - Web of Science (2016): Indexed yes
  - BFI (2015): BFI-level 1
  - Scopus rating (2015): SJR 0.427 SNIP 0.759 CiteScore 0.99
  - BFI (2014): BFI-level 1
Melt textured (YBa$_2$Cu$_3$O$_{7-δ}$)$_{1-x}$–(PrBa$_2$Cu$_3$O$_{7-δ}$)$_x$ composites (x=0.00 and x=0.05) were grown using the top seeding method. The effect of the PrBa$_2$Cu$_3$O$_{7-δ}$ phase on the growth process and the modification of the microstructure as well as on the physical properties was analyzed. X-ray analyses indicated that both pure and Pr-doped samples present an orthorhombic superconducting phase. From resistivity measurements for YBa$_2$Cu$_3$O$_{7-δ}$ and (YBa$_2$Cu$_3$O$_{7-δ}$)$_{0.95}$–(PrBa$_2$Cu$_3$O$_{7-δ}$)$_{0.05}$ samples, the $T_c$ did not change and was around 90.5 K. However, from magnetic measurements, the superconductivity was observed in critical temperatures $T_c=92.9$K and 92.4K for YBa$_2$Cu$_3$O$_{7-δ}$ and (YBa$_2$Cu$_3$O$_{7-δ}$)$_{0.95}$–(PrBa$_2$Cu$_3$O$_{7-δ}$)$_{0.05}$ samples, respectively. The YBa$_2$Cu$_3$O$_{7-δ}$ sample showed higher critical current densities than those shown by the (YBa$_2$Cu$_3$O$_{7-δ}$)$_{0.95}$–(PrBa$_2$Cu$_3$O$_{7-δ}$)$_{0.05}$ sample, with values of $J_c=5.85\times10^5$ A/cm$^2$ and $4.72\times10^5$ A/cm$^2$, respectively. This paper also discusses the importance of Pr substitution on nano- and micro-meter scales to enhance $J_c(H)$. 

Original language: English

MgB$_2$, Doping, Carbon, Potassium, K$_2$CO$_3$

DOIs: 10.1016/j.physc.2018.03.012

Publication: Research - peer-review › Journal article – Annual report year: 2018
Defect states and room temperature ferromagnetism in cerium oxide nanopowders prepared by decomposition of Ce-propionate

Four batches of cerium oxide powders (with nanocrystallite size of 6.9nm–572nm) were prepared from four precursor nanopowders by thermal decomposition of Ce-propionate and annealing in air between 250°C–1200°C for 10min–240min. Ceria formation reactions, structure, vibrational, luminescence and magnetic properties were investigated by differential scanning calorimetry, x-ray diffraction, electron microscopy, infrared spectroscopy, photoluminescence and SQUID. All the samples exhibit room temperature ferromagnetism, RTFM, (with coercivity, $H_c$, of 8Oe - 121Oe and saturation magnetization, $M_s$, of up to $6.7\times10^{-3}$emu/g) and a broad defect-related photoluminescence, PL, emission in the visible range. The samples derived from the same precursor show $M_s$ proportional to the peak area of defect-related PL emission whereas this is not valid for the samples derived from the different precursors. An improvement of ferromagnetism and intensity of defect-related PL emission was observed when annealing the products in which nanocrystalline cerium oxide coexists with Ce-oxcarbonate traces, Ce$_2$O$_2$CO$_3$. The experimental results were explained based on the following considerations: room temperature ferromagnetism was induced by the defective ceria with high concentration of oxygen vacancies generated by decomposition of Ce-propionate; oxygen vacancies of the starting precursor nanopowders could be redistributed (at the surfaces/grain boundaries, GBs) upon heating under conditions that promote an inert local environment; the decomposition of Ce$_2$O$_2$CO$_3$residues can provide an excess of oxygen vacancies at the nanoparticles surfaces or GBs, which can induce or enhance ferromagnetism; surfaces/GBs rather than bulk defects appear responsible for RTFM – this can explain the (often reported in literature) inconsistency between oxygen vacancies concentration and $M_s$.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, National Institute of Materials Physics
Authors: Mihalache, V. (Ekstern), Grivel, J. C. (Intern), Secu, M. (Ekstern)
Pages: 121-133
Publication date: 2018
Main Research Area: Technical/natural sciences
Deposition of highly oriented (K,Na)NbO₃ films on flexible metal substrates

In view of developing flexible, highly textured Pb-free piezoelectric thin films, (K,Na)NbO₃ was deposited by chemical solution deposition on cube-textured Ni-W alloy substrates. After heat treatment, a strong (001) out-of-plane preferential orientation is created in the (K,Na)NbO₃ layer, which also exhibits a sharp in-plane texture with $45^\circ$-rotated epitaxial relation to the substrate. The microstructure of the film is strongly dependent on the heat treatment temperature; submicrometer grains versus up to 2μm long particles forming at 600°C and 900°C respectively. $K_4Nb_8O_{17}$ and $(K_{1-x}Na_x)_{2}Nb_4O_{11}$ impurity phases were identified depending on the processing temperature.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Imaging and Structural Analysis, Ceramic Engineering & Science
Authors: Grivel, J. (Intern), Thydén, K. (Intern), Bowen, J. R. (Intern), Bjørnetun Haugen, A. (Intern)
Pages: 7-10
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information
Journal: Thin Solid Films
Volume: 650
ISSN (Print): 0040-6090
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 1.91 SJR 0.617 SNIP 0.864
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.83 SJR 0.639 SNIP 0.881
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.68 SNIP 0.923 CiteScore 1.84
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.725 SNIP 1.075 CiteScore 1.94
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.814 SNIP 1.195 CiteScore 2
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.897 SNIP 1.153 CiteScore 1.86
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 0.995 SNIP 1.323 CiteScore 2.13
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.132 SNIP 1.224
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.127 SNIP 1.213
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.182 SNIP 1.275
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.146 SNIP 1.192
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.142 SNIP 1.317
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.179 SNIP 1.227
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.201 SNIP 1.292
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.259 SNIP 1.281
Scopus rating (2002): SJR 1.036 SNIP 1.14
Scopus rating (2001): SJR 1.046 SNIP 1.032
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 0.929 SNIP 0.928
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 0.9 SNIP 0.865
Original language: English
Piezoelectric materials, Thin films, Sol-gel preparation, Texture
DOIs:
10.1016/j.tsf.2018.02.008
Source: Findit
Source-ID: 2396402365
Publication: Research - peer-review › Journal article – Annual report year: 2018
Design and testing of a heat transfer sensor for well exploration tools

The exploration of oil, gas, and geothermal wells is moving towards increasingly harsher downhole environments, requiring more and more advanced drilling and intervention tools. The high downhole temperatures threaten the correct functionality of intervention equipment and of standard downhole electronics, which cannot withstand temperatures above 150°C for an extended period of time. Thermal management of downhole electronics therefore requires critical and accurate knowledge of the thermal interaction between the downhole tools and the wellbore environment for correct tool design, intervention planning and operation. In this work, we present the design, modelling and testing of a sensor for downhole tools that can determine the heat transfer rate between the tool and the harsh downhole environment. An experimental flow loop was used to simulate the interaction between the sensor and the well fluid, and to calibrate the sensor in the range of heat transfer coefficients 0–1000W/m²K. Good agreement between model predictions and experimental results was obtained with average and maximum errors of ∼3% and ∼10%, respectively. A sensitivity of up to 8.7mV/(W/m²K) was measured and a response time of about 11s was obtained over a 25% change in the fluid velocity.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Energy Systems Analysis, Just Consulting IVS, Development & Engineering
Authors: Soprani, S. (Intern), Just Nørgaard, A. (Ekstern), Nesgaard, C. (Ekstern), Engelbrecht, K. (Intern)
Pages: 887-897
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information
Journal: Applied Thermal Engineering
Volume: 141
ISSN (Print): 1359-4311
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 4.14 SJR 1.505 SNIP 1.837
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.78 SJR 1.438 SNIP 1.851
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.683 SNIP 1.884 CiteScore 3.32
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.539 SNIP 2.187 CiteScore 3.16
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.466 SNIP 2.469 CiteScore 3.31
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.492 SNIP 2.422 CiteScore 2.7
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.338 SNIP 2.186 CiteScore 2.83
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.385 SNIP 2.012
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.393 SNIP 2.105
Design of Nickel-based cation-disordered rock-salt oxides: The effect of transition metal (M = V, Ti, Zr) substitution in LiNi$_{0.5M0.5}$O$_2$ binary systems

Cation-disordered oxides have been ignored as positive electrode material for a long time, due to structurally limited lithium insertion/extraction capabilities. In this work, a case study is carried out on nickel based cation-disordered Fm-3m LiNi$_{0.5M0.5}$O$_2$ positive electrode materials. The present investigation targets tailoring the electrochemical properties of nickel based cation-disordered rock-salt by electronic considerations. The compositional space for binary LiM$^+3$O$_2$ with metals active for +3/+4 redox couples is extended to ternary oxides of LiA$_0.5$B$_0.5$O$_2$ with A=Ni$^{+2}$ and B=Ti$^{+4}$, Zr$^{+4}$ and V$^{+4}$ in order to assess the impact of the different transition metal in the isostructural oxides. The direct synthesis of various new unknown ternary nickel based Fm-3m cation-disordered rock-salt positive electrode materials is presented with a particular focus on the LiNi$_{0.5V0.5}$O$_2$ system. This positive electrode material for Li ion batteries displays an average voltage of ~2.55 V and a high discharge capacity of 264 mAh/g corresponding to 0.94 Li. For appropriate cut-off voltages, a long cycle life is achieved. The charge compensation mechanism is probed by XANES, confirming the reversible oxidation and reduction of V$^4+/V^5+$. The enhancement in the electrochemical performances within the presented compounds stresses the importance of mixed cation-disordered transition metal oxides with different electronic configuration.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Imaging and Structural Analysis, Helmholtz Institute Ulm, Karlsruhe Institute of Technology KIT, Southern Federal University, Russian National Research Centre Kurchatov Institute
Authors: Cambaz, M. A. (Ekstern), Vinayan, B. P. (Ekstern), Euchner, H. (Ekstern), Johnsen, R. E. (Intern), Guda, A. A. (Ekstern), Mazilkin, A. (Ekstern), Rusalev, Y. V. (Ekstern), Trigub, A. L. (Ekstern), Gross, A. (Ekstern), Fichtner, M. (Ekstern)
Pages: 21957-21964
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information
Journal: A C S Applied Materials and Interfaces
Volume: 10
Issue number: 26
ISSN (Print): 1944-8244
Ratings:
- BFI (2018): BFI-level 2
- Web of Science (2018): Indexed yes
- BFI (2017): BFI-level 1
- Scopus rating (2017): CiteScore 8.15 SJR 2.784 SNIP 1.543
- Web of Science (2017): Indexed yes
- BFI (2016): BFI-level 1
Design of Thermal Systems Using Topology Optimization

The goal of this thesis is to apply topology optimization to the design of different thermal systems such as heat sinks and heat exchangers in order to improve the thermal performance of these systems compared to conventional designs. The design of thermal systems is a complex task that has traditionally relied on experience, intuition, and trial and error approaches. Topology optimization, in contrast, allows for a systematic optimization of such systems and the identification of intuitive and unexpected geometries. Both numerical optimizations and, to a lesser extent, experimental validations of optimized designs are presented within this thesis. The main contribution of the thesis is the development of several numerical optimization models that are applied to different design challenges within thermal engineering.

Topology optimization is applied in an industrial project to design the heat rejection system of a robotic downhole oil well intervention tool and an optimized prototype is built that can operate in environments of 200°C instead of 175°C, opening a new market for the company. A similar model is used in a different project to optimize the heat sink of a commercial tablet. The design of 3D printed dry-cooled power plant condensers using a simplified thermodynamic topology optimization model is presented in another study. A benchmarking of the optimized geometries against a conventional heat exchanger design is conducted and the topology-optimized designs show a superior performance. A thermodynamic topology optimization heat sink model is applied to the design of forced convection air-cooled heat sinks. Two topology optimized designs are exemplarily benchmarked against a size-optimized parallel fin heat sink and an up to 13% lower thermal resistance is found to be realized by the topology optimization. The design of cross-flow heat exchangers using thermodynamic topology optimization is presented in another work. This novel approach can explicitly solve the Navier-Stokes equations and capture the heat transfer in both fluids at a low computational cost.

Lastly, the fabrication and experimental validation of different topology-optimized heat transfer devices is summarized. The developed robotic downhole tool prototypes are successfully tested in the laboratory under conditions similar to those in boreholes. Two optimized commercial tablet heat sinks are manufactured, mounted in the device, and experimentally compared to an unoptimized heat sink. Moreover, the fabrication and experimental benchmarking of 3D optimized natural convection heat sink designs is presented. Investment casting using 3D stereolithography printed patterns is used to fabricate different heat sink designs and this technology is demonstrated to be promising for the fabrication of topology-optimized metal parts.

General information
Developing Smart Islands in the Adriatic Sea

Croatia is an EU member country which has 1244 islands in the Adriatic Sea. Only 50 islands are populated with significant depopulation in 20th century so number of people living on the islands decreased from 173,263 people in 1900 to 124,955 in 2011. Besides decrease in population certain traditional economy sectors such as agriculture, fishery and shipbuilding also decreased in the volume but on the other side tourism and related activities had significant increase. The tourism puts high stress on all resources on the islands, infrastructure and environment during the summer months. Due to climate change the problems with resources are increasing at an anticipated rate so islands are developing many strategies to mitigate and adopt to the climate change while preserving the environment. Although, there were many studies and pilot projects from the northern islands to the southmost islands in Adriatic Sea how to achieve sustainable, low carbon and 100% renewable energy systems they were never developed under the same umbrella or general policy and strategy. Currently, there are two main movements in the EU that organise islands and try to ensure them more sustainable future. Smart Islands Initiative is bottom up initiative of island local and regional governments while Clean energy for EU islands is top-down initiative of European commission and 14 EU member states. The paper presents analysis of historical and current studies on development of sustainable islands in the Adriatic Sea and provides the context for use of methods and tools for development of Smart Islands.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Energy Systems Analysis, Centre for IT-Intelligent Energy Systems in Cities, Regional Energy Agency Kvarner, University of Zagreb, SDEWES Centre
Authors: Krajačić, G. (Ekstern), Jardas, D. (Ekstern), Duć, N. (Ekstern), Dobravec, V. (Ekstern), Pfeifer, A. (Ekstern), Matak, N. (Ekstern), Dominkovic, D. F. (Intern), Ban, M. (Ekstern)
Publication date: 2018

Host publication information
Main Research Area: Technical/natural sciences
Conference: 1st Latin American Conference on Sustainable Development of Energy, Water and Environment Systems, Rio de Janeiro, Brazil, 28/01/2018 - 28/01/2018
Publication: Research - peer-review › Article in proceedings – Annual report year: 2018

Development of high temperature mechanical rig for characterizing the viscoplastic properties of alloys used in solid oxide cells

Analyzing the thermo-mechanical reliability of solid oxide cell (SOC) stack requires precise measurement of the mechanical properties of the different components in the stack at operating conditions of the SOC. It is challenging to precisely characterize the time dependent deformational properties of metallic components in the SOC stacks at the required level of stress and operational conditions (high temperature and controlled atmosphere). This work presents an improved methodology for characterizing the time dependent or viscoplastic properties of metallic alloys used in SOC stacks at high temperature and in controlled atmosphere. The methodology uses a mechanical loading rig designed to apply variable as well as constant loads on samples within a gas-tight high temperature furnace. In addition, a unique remotely installed length measuring setup involving laser micrometer is used to monitor deformations in the sample. Application of the methodology is exemplified by measurement of stress relaxation, creep and constant strain rate behaviors of a high temperature alloy used in the construction of SOC metallic interconnects at different temperatures. Furthermore, measurements using the proposed methodology are also verified with literature and experiments conducted using other machines.
DFT study of stabilization effects on N-doped graphene for ORR catalysis

Noble metal free catalysts, such as N-doped graphene, have drawn a lot of attention as a promising replacement for platinum in low temperature fuel cells. Computational prediction of catalytic activity requires accurate description of the
oxygen reduction reaction (ORR) intermediates adsorption energies. Two stabilizing effects, immanently present in experimental ORR setups with basal plane N-doped graphene catalyst, are studied systematically by means of density functional theory. Distant nitrogen with no adsorbates on neighboring carbon atoms selectively stabilizes *O and *O2 adsorbates. Water solvation stabilizes all ORR intermediates, having a greater impact on *O and *O2, than on *OH and *OOH, in contrast to metal and oxide catalysts. Synergistic stabilization of *O caused by both effects reaches remarkably a high value of 1.5 eV for nitrogen concentrations above 4.2% N. Such a strong effect is explained by a high reactivity of *O and *O2, which possess empty O(sp) states. At 6.25% N, the reaction environment is found to comprise *O and free nitrogen spectators. Finally, strong *O solvation is found to be present in a broader class of systems, comprising all materials where the ORR occurs on a 2nd row element. Including at least a single explicit water layer is paramount to achieve the correct description of the ORR intermediates adsorption energies on these materials.

**General information**

State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials
Authors: Reda, M. (Intern), Hansen, H. A. (Intern), Vegge, T. (Intern)
Number of pages: 8
Pages: 118-125
Publication date: 2018
Main Research Area: Technical/natural sciences
Direct Demonstration of the Emergent Magnetism Resulting from the Multivalence Mn in a LaMnO$_3$ Epitaxial Thin Film System

Atomically engineered oxide heterostructures provide a fertile ground for creating novel states, for example, a 2D electron gas at the interface between two oxide insulators, giant thermoelectric Seebeck coefficient, emergent ferromagnetism from otherwise nonmagnetic components, and colossal ionic conductivity. Extensive research efforts reveal that oxygen deficiency or lattice strain play an important role in determining these unexpected properties. Herein, by studying the abrupt presence of robust ferromagnetism (up to 1.5 $\mu_B$/Mn) in LaMnO$_3$-based heterostructures, the multivalence states of Mn that play a decisive role in the emergence of ferromagnetism in tfe otherwise antiferromagnetic LaMnO$_3$ thin films are found. Combining spatially resolved electron energy-loss spectroscopy, X-ray absorption spectroscopy, and X-ray magnetic circular dichroism techniques, it is determined unambiguously that the ferromagnetism results from a conventional Mn$^{3+}$-O-Mn$^{4+}$ double-exchange mechanism rather than an interfacial effect. In contrast, the magnetic dead layer of 5 unit cell in proximity to the interface is found to be accompanied with the accumulation of Mn$^{2+}$ induced by electronic reconstruction. These findings provide a hitherto-unexplored multivalence state of Mn on the emergent magnetism in undoped manganite epitaxial thin films, such as LaMnO$_3$ and BiMnO$_3$, and shed new light on all-oxide spintronic devices.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, University of London, Nanjing University, Technical University of Denmark, University of California, Irvine
Pages: 1-9
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information
Journal: Advanced Electronic Materials
Volume: 4
Issue number: 6
Article number: 1800055
Ratings:
Web of Science (2018): Indexed yes
Scopus rating (2017): CiteScore 4.33 SJR 2.129 SNIP 1.133
Web of Science (2017): Indexed Yes
Scopus rating (2016): CiteScore 1.98 SJR 2.564 SNIP 0.936
Original language: English
DOIs:
Distinct Nature of Static and Dynamic Magnetic Stripes in Cuprate Superconductors

We present detailed neutron scattering studies of the static and dynamic stripes in an optimally doped high-Temperature superconductor, La$_2$CuO$_{4+y}$. We observe that the dynamic stripes do not disperse towards the static stripes in the limit of vanishing energy transfer. Therefore, the dynamic stripes observed in neutron scattering experiments are not the Goldstone modes associated with the broken symmetry of the simultaneously observed static stripes, and the signals originate from different domains in the sample. These observations support real-space electronic phase separation in the crystal, where the static stripes in one phase are pinned versions of the dynamic stripes in the other, having slightly different periods. Our results explain earlier observations of unusual dispersions in underdoped La$_{2-x}$Sr$_x$CuO$_4$ (x=0.07) and La$_{2-x}$Ba$_x$CuO$_4$ (x=0.095).

General information

State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Department of Energy Conversion and Storage, Electrofunctional materials, Technical University of Denmark, University of Connecticut, University of Copenhagen, Institut Max von Laue-Paul Langevin
Authors: Jacobsen, H. (Ekstern), Holm, S. L. (Ekstern), Lăcătușu, M. E. (Ekstern), Rømer, A. T. (Ekstern), Bertelsen, M. (Ekstern), Boehm, M. (Ekstern), Toft-Petersen, R. (Intern), Grivel, J. (Intern), Emery, S. B. (Ekstern), Udby, L. (Ekstern), Wells, B. O. (Ekstern), Lefmann, K. (Ekstern)
Number of pages: 5
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information
Journal: Physical Review Letters
Volume: 120
Issue number: 3
Article number: 037003
ISSN (Print): 0031-9007
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 7.58 SJR 3.622 SNIP 2.464
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 6.33 SJR 4.196 SNIP 2.61
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 4.656 SNIP 2.538 CiteScore 5.76
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 5.232 SNIP 2.71 CiteScore 6.62
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 5.675 SNIP 2.781 CiteScore 7.46
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 6.292 SNIP 2.867 CiteScore 7.19
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 6.314 SNIP 2.905 CiteScore 7.02
ISI indexed (2011): ISI indexed yes
Effect of dimethyl carbonate (DMC) on the electrochemical and cycling properties of solid polymer electrolytes (PVP-MSA) and its application for proton batteries

Proton-conducting polymer electrolyte systems (PVP-MSA), with polyvinylpyrrolidone as a host polymer and methanesulfonic acid as a proton donor, were prepared by a facile solution-cast technique. The effects of plasticizer, dimethyl carbonate, on the electrical and electrochemical properties of PVP-MSA complexes were plausibly investigated for the first time. The complexation behaviors of both plasticized and unplasticized polymer electrolyte systems were confirmed with the aid of Fourier transform infrared spectroscopy. The conductivity values were found to be enhanced due to the addition of DMC, and a maximum value of $3.27 \times 10^{-5}$ S/cm was achieved. The ionic transport number values were found to be in the range of 0.96–0.99. The discharge analysis suggested that the proton battery constructed with the plasticized polymer electrolyte showed better performance compared to that constructed with the unplasticized polymer electrolyte, which in turn means it could be utilized as a promising candidate for primary proton batteries.
Effect of pre-oxidation on the oxidation resistance of Crofer 22 APU
The ferritic stainless steel Crofer 22 APU is attractive for the use as interconnects in solid oxide fuel cell stacks. The oxidation rate of this alloy in air at 800°C was reduced by pre-oxidation at higher temperatures in either air or N₂-9%H₂-1%H₂O. Conversely, the oxidation rate increased when the alloy grain size was increased by heat-treating in H₂ (pO₂∼10⁻² atm). In all cases the scale formed on Crofer 22 APU consisted of an outer (Mn,Cr)₃O₄ layer, an inner Cr₂O₃ layer and sub-scale MnCr₂O₄ nodules that preferentially formed at alloy grain boundaries.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Norwegian University of Science and Technology
Authors: Talic, B. (Intern), Molin, S. (Intern), Hendriksen, P. V. (Intern), Lein, H. L. (Ekstern)
Pages: 189-199
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information
Journal: Corrosion Science
Volume: 138
ISSN (Print): 0010-938X
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 5.15 SJR 1.846 SNIP 2.252
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 5.19 SJR 1.891 SNIP 2.448
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.907 SNIP 2.781 CiteScore 5.62
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.865 SNIP 2.993 CiteScore 5.08
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.594 SNIP 2.97 CiteScore 4.57
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.499 SNIP 2.751 CiteScore 4.3
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.396 SNIP 2.75 CiteScore 4.26
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.396 SNIP 2.512
Web of Science (2010): Indexed yes
Effect of spherical porosity on co-fired dense/porous zirconia bi-layers cambering

Geometrical instability leading to cambering is recorded during co-sintering of zirconia dense/porous bi-layered planar structures. Sintering strain in the bi-layers rises mainly from mismatch between the different porosity volume fractions at the layers and their interface. In this paper, we analyze the model case of dense tapes of 8 mol% Y2O3-stabilized ZrO2 laminated on ca. 400 μ thick 3 mol% Y2O3-doped zirconia porous tapes, with homogenous spherical porosity of 13 vol%, 46 vol%, and 54 vol%. Sintering stress during densification is evaluated from the shrinkage rates and viscoelastic behavior during sintering by thermo-mechanical analysis, using cyclic loading dilatometry. The camber development of the bi-layers is measured by in-situ optical dilatometry. In accordance with the model prediction, cambering can be controlled tuning the porosity while achieving a synergetic effect between densification and formation of open porosity at the bilayers.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Mixed Conductors, Universidade Federal do ABC
Authors: Teocoli, F. (Intern), Marani, D. (Ekstern), Kiebach, W. (Intern), Esposito, V. (Intern)
Pages: 173-179
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of the European Ceramic Society
Volume: 38
Issue number: 1
ISSN (Print): 0955-2219
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 3.55 SJR 1.068 SNIP 1.698
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.25 SJR 1.142 SNIP 1.888
Web of Science (2016): Indexed yes
Effect of the sol-gel conditions on the morphology and SCR performance of electrospun V-W-TiO₂ catalysts

V-W-TiO₂ catalysts are prepared as nanofibers for the removal of the NOx in exhausts via the NH₃ Selective Catalytic Reduction (SCR) method. By combining electrospinning and soft chemistry, materials are processed as nanofibers with the catalytic components (e.g., V₂O₅-WO₃) incorporated as dopants into the supporting anatase phase (e.g., TiO₂). The conditions for the chemical synthesis were investigated by varying the molar ratios between titanium alkoxide (tetraisopropoxide) and the chelating agent (acetic acid). Catalytic characterization clearly shows a impact of the starting precursor coordination on the final nanostructure, and thus on the catalytic performances. Superior NOx conversion is obtained for nanofibers formed by high coordination level, i.e., [Acetic acid]/[Ti cation]>2, with high stability and control over the processing route.
Effects of accelerated degradation on metal supported thin film-based solid oxide fuel cell
A thin film-based solid oxide fuel cell is deposited on a Ni-based metal porous support by pulsed laser deposition with a multi-scale-graded microstructure design. The fuel cell, around 1 μm in thickness, is composed of a stabilized-zirconia/doped-ceria bi-layered dense electrolyte and nanostructured Ni-stabilized zirconia and La0.6Sr0.4CoO3 electrodes as the anode and cathode, respectively. The cell is tested at intermediate temperatures (600–650 °C) with the aim to discern the degradation mechanisms occurring in the cell under accelerated conditions. Under open circuit conditions, electrochemical performances are steady, indicating the stability of the cell. Under electrical load, a progressive degradation is activated. Post-test analysis reveals both mechanical and chemical degradation of the cell. Cracks and delamination of the thin films promote a significant nickel diffusion and new phase formation. Signs of elemental distribution at low temperature are detected throughout the cell, indicating a combination of low energy surface elemental interdiffusion and electromigration effects.

Effects of Zr Doping on Magnetic and Structural Properties of DyBa2(Cu1−x−Zrx)3O7−δ Thin Films
DyBa2(Cu1−x−Zrx)3O7−δ thin films (with x = 0.00, 0.02, 0.04, and 0.06) were synthesized using the chemical solution deposition method on single crystalline LaAlO3 substrates. Effects resulting from Zr doping were investigated by means of magnetic and structural measurements. X-ray diffraction analysis demonstrated a strong c-axis orientation in the DyBa2(Cu1−x−Zrx)3O7−δ thin films, with only minor reflections due to the presence of Dy2O3 and BaZrO3 phases. Narrow transitions with Δ Tc ranging from 1 to 2 K for samples with x = 0.00 and 0.06, respectively, were observed in ac magnetic
susceptibility curves, where the nondoped sample demonstrated the highest T onsetc of 91.7 K compared to the Zr-doped samples. Critical current densities Jc of the thin films were obtained from magnetization loop measurements with applied magnetic fields up to 6 T and by employing the Bean model. The sampled doped with 4% Zr exhibited the highest Jc value (Jc = 3.5 MA/cm², self-field, 77 K) in the low field range and we, in general, observed that Zr-doped films demonstrated higher values compared to the pure sample. Pinning force plots (Fp versus B) reveal a significant improvement over the magnetic field range investigated of the maximum pinning force for Zr-doped samples. We found FMaxp = 1.7 GN/m³ and 3.8 GN/m³ for pure and 6% Zr samples, respectively. Analysis based on the Dew-Hughes model shows that normal surface pinning is the dominating pinning mechanism.

**General information**

State: Published  
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Department of Physics  
Authors: Opata, Y. A. (Intern), Wulff, A. C. (Intern), Hansen, J. O. B. (Ekstern), Grivel, J. (Intern)  
Number of pages: 4  
Publication date: 2018  
Main Research Area: Technical/natural sciences

**Publication information**

Journal: IEEE Transactions on Applied Superconductivity  
Volume: 28  
Issue number: 4  
Article number: 8000804  
ISSN (Print): 1051-8223  
Ratings:  
BFI (2018): BFI-level 1  
Web of Science (2018): Indexed yes  
BFI (2017): BFI-level 1  
Scopus rating (2017): CiteScore 1.45 SJR 0.408 SNIP 0.962  
Web of Science (2017): Indexed yes  
BFI (2016): BFI-level 1  
Scopus rating (2016): CiteScore 1.42 SJR 0.398 SNIP 1.145  
Web of Science (2016): Indexed yes  
BFI (2015): BFI-level 1  
Scopus rating (2015): SJR 0.403 SNIP 1.06 CiteScore 1.27  
Web of Science (2015): Indexed yes  
BFI (2014): BFI-level 1  
Scopus rating (2014): SJR 0.478 SNIP 1.13 CiteScore 0.83  
Web of Science (2014): Indexed yes  
BFI (2013): BFI-level 1  
Scopus rating (2013): SJR 0.443 SNIP 1.156 CiteScore 1.32  
ISI indexed (2013): ISI indexed yes  
Web of Science (2013): Indexed yes  
BFI (2012): BFI-level 1  
Scopus rating (2012): SJR 0.555 SNIP 1.274 CiteScore 1.11  
ISI indexed (2012): ISI indexed yes  
BFI (2011): BFI-level 1  
Scopus rating (2011): SJR 0.368 SNIP 1.062 CiteScore 1.16  
ISI indexed (2011): ISI indexed yes  
Web of Science (2011): Indexed yes  
BFI (2010): BFI-level 1  
Scopus rating (2010): SJR 0.473 SNIP 1.065  
BFI (2009): BFI-level 1  
Scopus rating (2009): SJR 0.447 SNIP 1.021  
Web of Science (2009): Indexed yes  
BFI (2008): BFI-level 1  
Scopus rating (2008): SJR 0.884 SNIP 0.981  
Scopus rating (2007): SJR 0.629 SNIP 1.093  
Web of Science (2007): Indexed yes
Elastocaloric effect vs fatigue life: Exploring the durability limits of Ni-Ti sheets under pre-strain conditions for elastocaloric cooling

Structural fatigue is the major obstacle that prevents practical applications of the elastocaloric effect (eCE) in cooling or heat-pumping devices. Here, the eCE and fatigue behaviour of Ni-Ti plates are systematically investigated in order to define the fatigue strain limit and the associated eCE. Initially, the eCE was evaluated by measuring adiabatic temperature changes at different strain amplitudes and different mean strains along the loading and unloading transformation plateaus. By comparing the eCE with and without pre-strain conditions, the advantages of cycling an elastocaloric material at the mean strain around the middle of the transformation plateau were demonstrated. In the second part of this work, we evaluated the fatigue life at the mean strain of 2.25% at the loading plateau and at the unloading plateau after initial pre-straining up to 6% and 10%, respectively. It is shown that on polished samples, durable operation of $10^5$ cycles can be reached with a strain amplitude of 0.50% at the loading plateau, which corresponds to adiabatic temperature changes of approximately 5K. At the unloading plateau (after initial pre-strain of 10%), durable operation was reached at a strain amplitude of 1.00%, corresponding to adiabatic temperature changes of approximately 8K. The functional fatigue was analysed after the cycling and it is shown that once the sample has been stabilized there is no further degradation of the eCE, even after $10^5$ cycles. These results present guidelines for the design and operation of efficient and durable elastocaloric devices in the future.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, University of Ljubljana, Institute of Metals and Technology Ljubljana, SAES Getters S.p.A.
Authors: Tusek, J. (Ekstern), Zerovnik, A. (Ekstern), Cebron, M. (Ekstern), Brojan, M. (Ekstern), Zuzek, B. (Ekstern), Engelbrecht, K. (Intern), Cadelli, A. (Ekstern)
Pages: 295-307
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information
Journal: Acta Materialia
Volume: 150
ISSN (Print): 1359-6454
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 6.18 SJR 3.263 SNIP 2.737
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 5.67 SJR 3.21 SNIP 2.702
Web of Science (2016): Indexed yes
Electric field-assisted pressureless sintering gadolinium-, yttrium- and samarium-doped barium cerate

Gadolinium-, yttrium- and samarium-doped barium cerate compounds were sintered either conventionally at 1500°C or applying an electric field at 1200°C. The combined results of dilatometry and impedance spectroscopy measurements in electric field-assisted sintered specimens show substantial improvement of the electrical conductivity. Improved grain-to-grain contact and the thermal removal of depleted chemical species due to Joule heating at the space charge region are
proposed as the main mechanisms for the increase of both the grain boundary and the bulk electrical conductivities, respectively.
Electrochemical performances of LiNi$_{1-x}$MnxPO$_4$ (x=0.05–0.2) olivine cathode materials for high voltage rechargeable lithium ion batteries

This study demonstrated to synthesis of carbon-free lithium nickel phosphate (LiNiPO$_4$) and its analogue of manganese doped LiNi$_{1-x}$MnxPO$_4$ (x = 0.05–0.2) cathode materials by a facile polyol method and their suitability for use in high voltage lithium ion batteries (LIBs). The physicochemical properties were analyzed using X-ray diffraction, Fourier transform infra-red, Raman, field emission scanning electron microscopy (FE-SEM), energy dispersive analysis by X-ray (EDX), and electrochemical studies. FE-SEM showed that the spherical shape particles were uniformly distributed on the surface and EDX confirmed the presence of all the elements in the LiNi$_{1-x}$MnxPO$_4$ nanostructure. Substitution of Mn dopants with LiNiPO$_4$ significantly improved the electrical and electrochemical performances for LiNi$_{1-x}$MnxPO$_4$ (x = 0.05–0.2) cathodes. The highly conducting LiNi$_{1-x}$MnxPO$_4$ (x = 0.1) cathode exhibited initial discharge capacity of 94.2 mA h g$^{-1}$ at C/4 rate, and 62% capacity retention after 100 cycles between 2.8 and 5.6 V. These features promote LiNi$_{1-x}$MnxPO$_4$ as a suitable cathode material for high voltage LIBs.

General information

State: Published
Organisations: Department of Energy Conversion and Storage, Electrochemical Materials and Interfaces, K. Ramakrishnan College of Technology, Dongguk University, SRM University, St. Mother Theresa Engineering College
Authors: Karthikprabhu, S. (Ekstern), Karuppasamy, K. (Ekstern), Vikraman, D. (Ekstern), Prasanna, K. (Intern), Maiyalagan, T. (Ekstern), Nichelson, A. (Ekstern), Kathalingam, A. (Ekstern), Kim, H. (Ekstern)
Pages: 435-444
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information
Journal: Applied Surface Science
Volume: 449
ISSN (Print): 0169-4332
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 4.22 SJR 1.093 SNIP 1.328
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.37 SJR 0.958 SNIP 1.221
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.89 SNIP 1.268 CiteScore 3.13
Electrochemical probing into the active sites of graphitic-layer encapsulated iron oxygen reduction reaction electrocatalysts

The graphitic-layer encapsulated iron-containing nanoparticles (G@Fe) have been proposed as a potential type of active and stable non-precious metal electrocatalysts (NPMCs) for the oxygen reduction reaction (ORR). However, the contribution of the encapsulated components to the ORR activity is still unclear compared with the well-recognized surface coordinated FeN/C structure. Using the strong complexing effect of the iron component with anions, cyanide (CN⁻) in alkaline and thiocyanate (SCN⁻) in acidic media, the metal containing active sites are electrochemically probed. Three representative catalysts are chosen for a comparison including the as-prepared encapsulated G@Fe, commercial Fe/N/C catalyst with iron–nitrogen coordinated surface functionalities and molecular iron phthalocyanine (FePc) containing well-defined structures and compositions. It was found that all samples showed significant shifts of half-wave potentials.
indicating that surface Fe coordinated sites in all cases. The G@Fe catalyst showed the weakest poisoning effect (the lowest shifts of half-wave potential) compared to the Fe/N/C and FePc catalysts in both electrolytes. These results could be explained that the encapsulated iron components influence the FeNₓ/C and/or NₓC surface functionality.

**General information**
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors
Authors: Zhong, L. (Intern), Jensen, J. O. (Intern), Cleemann, L. N. (Intern), Pan, C. (Intern), Li, Q. (Intern)
Pages: 24-30
Publication date: 2018
Main Research Area: Technical/natural sciences

**Publication information**
Journal: Science Bulletin
Volume: 63
Issue number: 1
ISSN (Print): 0309-7552
Original language: English
Encapsulated Fe catalysts, Oxygen reduction reaction, Ion poisoning, Active sites, NPMCs
DOI: 10.1016/j.scib.2017.11.017
Source: PublicationPreSubmission
Source-ID: 141974553
Publication: Research - peer-review › Journal article – Annual report year: 2018

**Electron mobility in oxide heterostructures: Topical review**
Next-generation integrated circuit devices based on transition-metal-oxides are expected to boast a variety of extraordinary properties, such as superconductivity, transparency in the visible range, thermoelectricity, giant ionic conductivity and ferromagnetism. However, the realisation of this so-called oxide electronics as well as the study of their unconventional physics is stalled by inferior carrier mobilities compared to conventional semiconductor materials. Over the past 10 years, bulk conducting oxides and oxide heterostructures with superior carrier mobilities have nonetheless seen significant progress. This progress is signifying the approaching era of oxide-based electronic circuits along with novel solid-state phenomena originating from the combination of hybridized oxygen p orbitals, transition-metal d orbitals and electronic correlations. Here, we review the recent advancements and results on high mobility oxide heterostructures based on SrTiO3 and ZnO as well as other prominent oxides.

**General information**
State: Published
Organisations: Electrofunctional materials, Department of Energy Conversion and Storage, Universite Paris-Sud
Authors: Trier, F. (Ekstern), Christensen, D. V. (Intern), Pryds, N. (Intern)
Number of pages: 23
Publication date: 2018
Main Research Area: Technical/natural sciences

**Publication information**
Volume: 51
Issue number: 29
ISSN (Print): 0022-3727
Article number: 293002
Published: yes
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 2.38 SJR 0.717 SNIP 1.011
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.07 SJR 1.135 SNIP 1.122
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.886 SNIP 1.25 CiteScore 2.1
Web of Science (2015): Indexed yes
Electron Mobility in $\gamma$-Al$_2$O$_3$/SrTiO$_3$

One of the key issues in engineering oxide interfaces for electronic devices is achieving high electron mobility. SrTiO$_3$-based interfaces with high electron mobility have gained a lot of interest due to the possibility of combining quantum phenomena with the many functionalities exhibited by SrTiO$_3$. To date, the highest electron mobility (140 000 cm$^2$/V s at 2 K) is obtained by interfacing perovskite SrTiO$_3$ with spinel $\gamma$-Al$_2$O$_3$. The origin of the high mobility, however, remains poorly understood. Here, we investigate the scattering mechanisms limiting the mobility in $\gamma$-Al$_2$O$_3$/SrTiO$_3$ at temperatures between 2 and 300 K and over a wide range of sheet carrier densities. For $T>$150 K, we find that the mobility...
is limited by longitudinal optical phonon scattering. For large sheet carrier densities (>8×10^{13} \text{ cm}^{-2}), the screened electron-phonon coupling leads to room-temperature mobilities up to μ∼12 \text{ cm}^2/\text{V s}. For 5 K

**General information**
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Bar-Ilan University, Universität Würzburg
Authors: Christensen, D. V. (Intern), Frenkel, Y. (Ekstern), Schütz, P. (Ekstern), Trier, F. (Intern), Wissberg, S. (Ekstern), Claessen, R. (Ekstern), Kalisky, B. (Ekstern), Smith, A. (Intern), Chen, Y. Z. (Intern), Pryds, N. (Intern)
Number of pages: 10
Publication date: 2018
Main Research Area: Technical/natural sciences

**Publication information**
Journal: Physical Review Applied
Volume: 9
Issue number: 5
Article number: 054004
ISSN (Print): 2331-7019
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 4.62 SJR 2.089 SNIP 1.406
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.83 SJR 2.449 SNIP 1.602
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SNIP 1.492 SJR 2.345 CiteScore 3.31
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
BFI (2013): BFI-level 1
Original language: English
Electronic versions:
GAO_Mobility_Article_vPostprint.pdf
DOIs:
10.1103/PhysRevApplied.9.054004
Source: FindIt
Source-ID: 2434573171
Publication: Research - peer-review › Journal article – Annual report year: 2018

Emergent ferromagnetism in an otherwise antiferromagnetic LaMnO3-based heterostructure attributable to the cation-vacancy-induced oxygen excess effect through direct observation of multivalence Mn is reported by Xuefeng Wang, Peng Wang, Yongbing Xu, Yunzhong Chen, and co-workers in article number 1800055. The ferromagnetism is mediated by the Mn3+–O–Mn4+ double-exchange mechanism. It provides a hitherto unexplored multivalence state of Mn on the emergent ferromagnetism in manganite thin films.

**General information**
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Nanjing University, University of London, College of Engineering and Applied Sciences; Nanjing University; Nanjing 210093 China
Number of pages: 1
Publication date: 2018

**Publication information**
Original language: English
Energy storage innovation challenge

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Forschungszentrum Jülich GmbH
Authors: Pedersen, A. S. (Intern), Linderoth, S. (Intern), Eichel, R. (Ekstern)
Pages: 99-109
Publication date: 2018

Host publication information
Title of host publication: Accelerating the clean energy revolution - perspectives on innovation challenges: DTU International Energy Report 2018
Publisher: Technical University of Denmark (DTU)
ISBN (Electronic): 978-87-93458-57-4
Chapter: 12
Main Research Area: Technical/natural sciences
Electronic versions:

Enhanced Oxygen Reduction Activity by Selective Anion Adsorption on Non-Precious-Metal Catalysts
Non-precious-metal catalysts (NPMC) are promising alternatives to platinum-based catalysts for the oxygen reduction reaction (ORR), which is the cathode reaction in fuel cells. In this paper, we focus on an iron–nitrogen–carbon (Fe/N/C) catalyst, in comparison to platinum, and investigate how these different types of catalysts behave toward selective anion poisoning. The catalysts are studied with respect to their ORR activity, using the rotating disk electrode (RDE) technique in aqueous HClO4, H2SO4, H3PO4, and HCl electrolytes, and the results are supported by density functional theory (DFT) calculations. We find that the ORR on the Fe/N/C catalyst is less affected by anion poisoning than platinum. Surprisingly, it is seen that phosphoric acid not only does not poison the Fe/N/C catalyst, but instead promotes the ORR; this finding is in sharp contrast to the poisoning effect observed on platinum. This is a highly important finding, as modern high-temperature proton exchange fuel cells (HT-PEMFCs) employ membranes consisting of phosphoric acid that is immobilized into a polybenzimidazole (PBI) matrix.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, University of Bern, University of Copenhagen
Authors: Holst-Olesen, K. (Ekstern), Reda, M. K. (Intern), Hansen, H. A. (Intern), Vegge, T. (Intern), Arenz, M. (Ekstern)
Number of pages: 9
Pages: 7104-7112
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information
Journal: ACS Catalysis
Volume: 8
ISSN (Print): 2155-5435
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 11.49 SJR 4.921 SNIP 2.113
Web of Science (2017): Indexed yes
Enhanced visible light catalytic activity of MoS2/TiO2/Ti photocathode by hybrid-junction

In photoelectrochemical (PEC) water splitting systems, crucial obstacles limiting their performance are poor charge carrier dynamics and high recombination rate of photoexcited electron hole pairs. Here, we report that this issue can be alleviated by engineering a hybrid-junction that is composed of homo- and hetero- junctions. This strategy is performed by facile hand-spraying MoS2 over the surface of a anatase/rutile homo-junction TiO2 film on the Ti substrate to further form a hybrid-junction photocathode. By applying this photocathode into PEC reactor, enhanced catalytic activity is achieved under visible light (AM1.5 illumination of 300W/m2) with hydrogen evolution reaction (HER) potential of −114mV versus reversible hydrogen electrode (RHE) at 10mA/cm2 and long-term stability of more than 10 times improvement comparing to ordinary electrode without the introduction of hybrid-junction. The hybrid-junction that effectively regulates charge separation and transfer pathways is proven to be responsible for the enhanced activity. As an novel exploration, this hybrid-junction system comprising of low-cost, efficient charge separation and transfer, and visible light responsivity offers a new path for relative materials to boost their PEC performance.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, University College of Southeast Norway, North China Electric Power University, Taiyuan University of Technology
Number of pages: 8
Pages: 416-423
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information
Journal: Applied Catalysis B: Environmental
Volume: 237
ISSN (Print): 0926-3373
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 10.92 SJR 3.152 SNIP 2.359
Web of Science (2017): Indexed yes
Enzyme immobilization on Inorganic Surfaces for Membrane Reactor Applications: Mass Transfer Challenges, Enzyme Leakage and Reuse of Materials

Enzyme immobilization is an established method for the enhancement of enzyme stability and reusability, two factors that are of great importance for industrial biocatalytic applications. Immobilization can be achieved by different methods and on a variety of carrier materials, both organic and inorganic. Inorganic materials provide the advantage of high stability and
long service life which, together with the prolonged service life of the immobilized enzyme, can benefit the process economy. However, enzyme immobilization and increased stability often come at the cost of decreased enzyme activity. The main challenges involved in the design of an efficient immobilized enzyme system is to obtain both retention of high enzyme activity, enhanced stability and reusability, which is a complicated task, given the many variables involved, and the large numbers of methods and materials available. Simultaneously, new carrier materials and morphologies are constantly being developed. An investigation of enzyme immobilization systems on inorganic materials, with special emphasis on inorganic membranes, has been conducted in order to evaluate the effects of the immobilization system on the enzyme properties upon immobilization, i.e., activity, stability and reusability. The main properties of the enzyme particles (carrier and membranes) and their effects on the success of immobilization are described here. Furthermore, the reuse of inorganic membranes as enzyme carriers has been investigated and the reported examples show high ability of regeneration. To the best of our knowledge, this is the first review on enzyme immobilization focusing on the three fundamental aspects to consider when dealing with the topic: catalytic properties, enzyme leakage and reusability.

Abbreviations: β-Gal: β‐d‐galactosidase; ADH: alcohol dehydrogenase; AFM: atomic force microscopy; APTES: 3‐aminopropyltriethoxysilane; APTMS: 3‐aminopropyltrimethoxysilane; BPA: bisphenol A; BSA: bovine serum albumin; CA: carbonic anhydrase; CALB: Candida antarctica lipase B; CD: circular dichroism; CDI: carbonyldimidazole; CLEA: cross‐linked enzyme aggregates; CLSM: confocal laser scanning microscopy; CNT: controlled pore glass; CRL: Candida rugosa lipase; DMeDMOS: dimethyldimethoxysilane; DRIFT: diffuse reflectance Fourier transform infrared; E2: 17β‐estradiol; EDC: N‐(3‐dimethylaminopropyl)‐N′‐ethylcarbodiimide hydrochloride; EDS: electron dispersive spectroscopy; FDH: formate dehydrogenase; FESEM: field emission scanning microscopy; FT‐IR: Fourier transform infrared spectroscopy; GA: glutaraldehyde; GCSZn: coal fly ashes glass‐ceramic zinc sulfate; GOD: glucose oxidase; GPS: 3‐(glycidyloxypropyl)trimethoxysilane; HDMI: hexamethylene diisocyanate; HRP: horseradish peroxidase; IEP: isoelectric point; IPTES: (3‐isocyanatopropyl)triethoxysilane; IR: infrared spectroscopy; LbL: layer‐by‐layer; MCP: metallic ceramic powder; MeTEOS: methyltriethoxysilane; MF: microfiltration; MML: Mucor miehei lipase; MNP: magnetic nanoparticle; MPTMS: 3‐mercaptopropyltrimethoxysilane; NHS: N‐hydroxysuccinimidyl; PAH: poly(allylamine hydrochloride); PEI: polyethyleneimine; PEG: polyethylene glycol; PES: polystyrene sulfonate; PTMS: phenyltriethoxysilane; RHOD: Rhizopus oryzae lipase; SCAD: Saccharomyces cerevisiae alcohol dehydrogenase; SDS: sodium dodecyl sulfate; SDS‐2: sodium dodecyl sulfonate; SEM: scanning electron microscopy; TEM: transmission electron microscopy; TLL: Thermomyces lanuginosa lipase; TVL: Trametes versicolor laccase; UF: ultrafiltration; VTMS: vinyltrimethylsiline

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, Department of Energy Conversion and Storage, Ceramic Engineering & Science, Electrofunctional materials
Pages: 2578-2607
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information
Journal: Advanced Synthesis and Catalysis
Volume: 360
Issue number: 14
ISSN (Print): 1615-4150
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 5.01 SJR 2.079 SNIP 0.935
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 2.416 SNIP 0.948 CiteScore 5.36
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 2.59 SNIP 1.102 CiteScore 6.07
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.339 SNIP 1.106 CiteScore 5.4
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 2.659 SNIP 1.106 CiteScore 5.56
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Evaluation of electrodeposited Mn-Co protective coatings on Crofer 22 APU steel

Interconnects used in Solid Oxide Cells stacks require protective coatings to lower their parabolic rate constant and block chromium evaporation (on the air side). In this work four different protective coatings on steel are evaluated for their high temperature corrosion resistance and electrical conductivity. A commercial electroplating process was used for the preparation of coatings with different Mn/Co ratios on Crofer 22 APU steel. Oxidation of samples was performed in air at 800°C for 1000 hours. Postmortem analysis of the coated samples was performed by scanning electron microscopy and x-ray diffractometry. Based on the results, influence of the Co/Mn ratio on the resulting corrosion properties are discussed. Parabolic rate constant of the coated samples is the lowest for the MnCo sample, whereas electrical resistance is the lowest for the Co sample, which has a corrosion rate similar to the not-coated alloys.
Experimental and numerical comparison of multi-layered La(Fe, Si, Mn)$_{13}\gamma$ active magnetic regenerators

We present an experimental and numerical comparison of epoxy bonded multi-layered La(Fe, Si, Mn)$_{13}\gamma$ active magnetic regenerators. First, no-load tests were performed on four regenerators with two layers of material and varying amounts of epoxy (from 1 wt. % to 4 wt. %) in order to find the amount of epoxy necessary to maintain the mechanical integrity of the regenerators. As the second part of the study, experimental results of two regenerators with five and nine layers are compared to predictions from the one-dimensional numerical model. A maximum temperature span, $\Delta T_{\text{span}}$, over 20 K was measured and it is effectively equal for both regenerators. The numerical modelling was generally in good agreement with experimental results.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Iowa State University, Vacuumschmelze GmbH & Co. KG
Authors: Navickaité, K. (Intern), Bez, H. N. (Ekstern), Lei, T. (Intern), Barcza, A. (Ekstern), Vieyra, H. (Ekstern), Bahl, C. (Intern), Engelbrecht, K. (Intern)
Pages: 322-330
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information
Journal: International Journal of Refrigeration
Volume: 86
ISSN (Print): 0140-7007
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 1.888 SJR 1.471 CiteScore 3.46
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.06 SJR 1.371 SNIP 1.607
Web of Science (2016): Indexed yes
Experimental investigation of different fluid flow profiles in a rotary multi-bed active magnetic regenerator device

A rotary multi-bed active magnetic regenerator (AMR) device was modified to allow testing different fluid flow waveforms, with different blow fractions (i.e. the fraction of the AMR cycle when there is fluid flow in the regenerators). The different values of blow fraction were generated using different cam rings that actuate the poppet valves at the inlet and outlet of the regenerators, controlling how long the valves stay open and the number of valves open at the same time. Results showed that smaller blow fractions yield higher values of temperature span for fixed flow rate and cooling capacity, but lower values of coefficient of performance for the same conditions. An analysis of the shaft and pumping powers showed that shorter blow fractions cause higher pressure drop and higher torque oscillations and mechanical vibrations. The highest value of second-law efficiency of 19.1% was obtained for the largest blow fraction tested (80%). Designs for magnetic refrigerators where the fluid flow waveform can change during operation are also discussed in this paper.
Extreme Reconfigurable Nanoelectronics at the CaZrO₃/SrTiO₃ Interface

Complex oxide heterostructures have fascinating emergent properties that originate from the properties of the bulk constituents as well as from dimensional confinement. The conductive behavior of the polar/nonpolar LaAlO₃/SrTiO₃ interface can be reversibly switched using conductive atomic force microscopy (c-AFM) lithography, enabling a wide range of devices and physics to be explored. Here, extreme nanoscale control over the CaZrO₃/SrTiO₃ (CZO/STO) interface, which is formed from two materials that are both nonpolar, is reported. Nanowires with measured widths as narrow as 1.2 nm are realized at the CZO/STO interface at room temperature by c-AFM lithography. These ultrathin nanostructures have spatial dimensions at room temperature that are comparable to single-walled carbon nanotubes, and hold great promise for alternative oxide-based nanoelectronics, as well as offer new opportunities to investigate the electronic structure of the complex oxide interfaces. The cryogenic properties of devices constructed from quasi-1D channels, tunnel barriers, and planar gates exhibit gate-tunable superconductivity, quantum oscillations, electron pairing outside of the superconducting regime, and quasi-ballistic transport. This newly demonstrated ability to control the metal–insulator transition at nonpolar oxide interface greatly expands the class of materials whose behavior can be patterned and reconfigured at extreme nanoscale dimensions.

General information

State: Accepted/In press
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, University of Pittsburgh
Authors: Chen, L. (Ekstern), Li, J. (Ekstern), Tang, Y. (Ekstern), Pai, Y. (Ekstern), Chen, Y. (Intern), Pryds, N. (Intern), Irvin, P. (Ekstern), Levy, J. (Ekstern)
Number of pages: 8
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information

Journal: Advanced Materials
Article number: 1801794
Ratings:
Web of Science (2018): Indexed yes
Scopus rating (2017): CiteScore 21.1
Scopus rating (2016): CiteScore 17.79
Scopus rating (2015): CiteScore 18.5
Scopus rating (2014): CiteScore 16.79
Scopus rating (2013): CiteScore 15.78
Scopus rating (2012): CiteScore 14.41
Scopus rating (2011): CiteScore 12.28
Original language: English
2D electron system, c-AFM lithography, Complex oxides, Quantum transport, Superconductivity
DOI: 10.1002/adma.201801794
Source: FindIt
Source-ID: 2436371589
Publication: Research - peer-review » Journal article – Annual report year: 2018

Fabricating eco-friendly nanocomposites of SiC with morphologically-different nano-carbonaceous phases

A route based on aqueous colloidal processing followed by liquid-phase assisted spark-plasma-sintering (SPS) is described for fabricating eco-friendly nanocomposites of SiC with nano-carbonaceous phases (nanotubes, nanoplatelets, or nanoparticles). To this end, the conditions optimizing the aqueous colloidal co-dispersion of SiC nanoparticles, Y₃Al₅O₁₂ nanoparticles (acting as sintering additives), and carbon nanotubes (CNTs), graphene oxide (GO) nanoplatelets, or
carbon black (CB) nanoparticles were first identified. Next, homogeneous powder mixtures were prepared by freeze-
drying, and densified by liquid-phase assisted SPS, thus obtaining nanocomposites of SiC with CNTs, reduced GO (rGO)
nanoplatelets, or pyrolized+graphitized CB (p+gCB) nanoparticles. It is also shown that these nanocomposites are dense
and have a high hardness of ~20GPa regardless of the nano-carbonaceous phase chosen, but are markedly tougher with
CNTs and rGO (i.e., with high aspect ratio nano-carbonaceous phases). Finally, arguments are provided for the
appropriate choice of nano-carbonaceous phases for engineering ceramic nanocomposites.
Fluctuation-induced conductivity in melt-textured Pr-doped YBa$_2$Cu$_3$O$_{7-\delta}$ composite superconductor

In this study, the effects of thermal fluctuations on the electrical conductivity in melt-textured YBa$_2$Cu$_3$O$_{7-\delta}$, Y$_{0.95}$Pr$_{0.05}$Ba$_2$Cu$_3$O$_{7-\delta}$, and (YBa$_2$Cu$_3$O$_{7-\delta}$)$_{0.95}$–(PrBa$_2$Cu$_3$O$_{7-\delta}$)$_{0.05}$ composite superconductor were considered. The composite superconductor samples were prepared through the top seeding method using melt-textured NdBa$_2$Cu$_3$O$_{7-\delta}$ seeds. The resistivity measurements were performed with a low-frequency, low-current AC technique in order to extract the temperature derivative and analyze the influence of the praseodymium ion on the normal superconductor transition and consequently on the fluctuation regimes. The results show that the resistive transition is a two-step process. In the normal phase, above the critical temperature, Gaussian and critical fluctuation regimes were identified, while below the critical temperature, in the regime near the approach to the zero-resistance state, the fluctuation conductivity diverges as expected in a paracoherent-coherent transition.
We report on the dielectric response of epitaxial BaSnO$_3$ films grown on Nb-doped SrTiO$_3$(001) substrates using a hybrid molecular beam epitaxy approach. Metal-insulator-metal capacitors were fabricated to obtain frequency- and temperature-dependent dielectric constant and loss. Irrespective of film thickness and cation stoichiometry, the dielectric constant obtained from Ba$_{1-x}$Sn$_{1-y}$O$_3$ films remained largely unchanged at 15-17 and was independent of frequency and temperature. A loss tangent of $\sim 1 \times 10^{-3}$ at 1 kHz $< f < 100$ kHz was obtained for stoichiometric films, which increased significantly with non-stoichiometry. Using density functional theory calculations, these results are discussed in the context of point defect complexes that can form during film synthesis.
Highly porous CeO₂ nanostructures prepared via combustion synthesis for supercapacitor applications

We report highly porous CeO₂ nanostructures (CeO₂ NSs) suitable for supercapacitor applications, synthesized using a fast and cost effective combustion approach. Due to its prominent valence states of Ce³⁺/Ce⁴⁺, CeO₂ has emerged as a promising pseudocapacitive material. The drawback of using CeO₂ as a supercapacitor electrode is its poor electrical conductivity. We overcame this drawback of CeO₂ by creating oxygen vacancies on its surface, which act to enhance its electrical conductivity. The physical interpretation of the as-synthesized CeO₂ NSs shows that they have dense active sites and diffusion pathways that enhance the performance of the electrode in a supercapacitor. Electrodes prepared using the synthesized CeO₂ NSs exhibited the initial specific capacitance of 134.6 F g⁻¹ and superior cycling stability of 92.5% after 1000 cycles at a constant current density of 1 A g⁻¹, indicating their potential suitability for use as efficient electrode for supercapacitor devices. The facile synthesis method used herein would help to reduce the cost and time required to synthesize CeO₂ particles and also would avoid the need to research and/or synthesize beneficial composite structures for enhancing the electrochemical properties of CeO₂ based electrodes.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Kyung Hee University
Authors: Kadirvelayutham, P. (Intern), Santhoshkumar, P. (Ekstern), Jo, Y. N. (Ekstern), Sivagami, I. N. (Ekstern), Kang, S. H. (Ekstern), Joe, Y. C. (Ekstern), Lee, C. W. (Ekstern)
Pages: 454-460
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information
Journal: Applied Surface Science
Volume: 449
ISSN (Print): 0169-4332
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 4.22 SJR 1.093 SNIP 1.328
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.37 SJR 0.958 SNIP 1.221
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.89 SNIP 1.268 CiteScore 3.13
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.948 SNIP 1.453 CiteScore 2.96
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.96 SNIP 1.475 CiteScore 2.78
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
High stability of benzotriazole and benzodithiophene containing medium band-gap polymer solar cell

The improvement of polymer solar cell stability is a challenge for the scientists and has significant implications commercially. In this study, we investigated the stability of a novel P-SBTBDT active material applied in an inverted type solar cell. Detailed stability experiments comprising shelf life, laboratory weathering and outdoor testing were carried out according to ISOS testing guidelines. Shelf life showed that P-SBTBDT solar cells were very stable after 840 h with encapsulation. Although accelerated weathering aging tests are very harsh, the devices remained stable after the burn-in phase with T50 from 700 to 840 h, with some P-SBTBDT solar cells did not reach T50 in the time span of the test. Degradation tests on the P-SBTBDT solar cells which were carried out under natural solar light indicated that T40 was reached after 840 h. The results of dark, light, damp and dry stability tests showed that most of the degradation was provoked by failure of the encapsulation. The experiments indicated that P-SBTBDT solar cells are sensitive to light and oxygen but are strikingly stable under humid conditions. Further developments for minimizing the degradation effects using UV-filters and better encapsulation are some of the necessary improvements in further research.

General information

State: Published

Organisations: Department of Photonics Engineering, Diode Lasers and LED Systems, Organic Energy Materials, Department of Energy Conversion and Storage, Middle East Technical University, Yildiz Technical University, TUBITAK


Pages: 433-444
High-Temperature Thermal Energy Storage for electrification and district heating

The present work describes development of a High Temperature Thermal Energy Storage (HT-TES) system based on rock bed technology.

A selection of rocks was investigated by thermal analysis in the range 20-800 °C. Subsequently, a shortlist was defined primarily based on mechanical and chemical stability upon thermal cycling. The most promising material consists of basalt, diabase, and magnetite, whereas the less suited rocks contain larger proportions of quartz and mica.

An HT-TES system, containing 1.5 m³ of rock pieces, was constructed. The rock bed was heated to 600 °C using an electric heater to simulate thermal charging from wind energy. After complete heating of the rock bed it was left fully charged for hours to simulate actual storage conditions. Subsequently the bed discharging was performed by leading cold air through the rock bed whereby the air was heated and led to an exhaust.

The results showed that HT-TES has a role to play in future, sustainable energy systems. A cost benefit analysis based on projected electricity prices for the Scandinavian region in 2035 showed that a business case is achievable.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Mixed Conductors, Polytchnical University of Milan, Aarhus University, Danish Energy Association, SEAS-NVE, Rockwool International, Energinet.dk
Number of pages: 12
Publication date: 2018
Main Research Area: Technical/natural sciences
Thermal energy, Rock bed, Storage, Minerals, Thermal properties, Economy
Source: PublicationPreSubmission
Source-ID: 147355907
Publication: Research - peer-review › Paper – Annual report year: 2018

High-temperature thermoelectric properties of Na- and W-Doped Ca₃Co₄O₉ system

The detailed crystal structures and high temperature thermoelectric properties of polycrystalline Ca₃₋₂ₓNa₂ₓCo₄₋ₓWₓO₉ (0 ≤ x ≤ 0.075) samples have been investigated. Powder X-ray diffraction data show that all samples are phase pure, with no detectable traces of impurity. The diffraction peaks shift to lower angle values with increase in doping (x), which is consistent with larger ionic radii of Na⁺ and W⁶⁺ ions. X-ray photoelectron spectroscopy data reveal that a mixture of Co²⁺, Co³⁺ and Co⁴⁺ valence states are present in all samples. It has been observed that electrical resistivity (ρ), Seebeck coefficient (S) and thermal conductivity (κ) are all improved with dual doping of Na and W in Ca₃Co₄O₉ system. A maximum power factor (PF) of 2.71 × 10⁻⁴ W m⁻¹ K⁻² has been obtained for x = 0.025 sample at 1000 K. The corresponding thermoelectric figure of merit (zT) for x = 0.025 sample is calculated to be 0.21 at 1000 K, which is ∼2.3 times higher than zT value of the undoped sample. These results suggest that Na and W dual doping is a promising approach for improving thermoelectric properties of Ca₃Co₄O₉ system.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrochemical Materials and Interfaces, Electrofunctional materials, Lahore University of Management Sciences (LUMS)
Authors: Hira, U. (Ekstern), Han, L. (Intern), Norman, K. (Intern), Christensen, D. V. (Intern), Pryds, N. (Intern), Sher, F. (Ekstern)
Pages: 12211–12221
Publication date: 2018
Main Research Area: Technical/natural sciences
Immunity of the Fe-N-C catalysts to electrolyte adsorption: phosphate but not perchloric anions

Non-precious metal catalysts (NPMCs), particularly the type based on carbon-supported FeNₓ functionalities (Fe-N-C) are a very promising material for replacing the rare and costly platinum-based catalysts in polymer electrolyte membrane fuel cells (PEMFCs). Evaluation of these materials is most often carried out, like for Pt-based catalysts, in dilute perchloric acid by assuming its non-adsorbing nature on the active sites. The assumption is however not true. In this work, a typical Fe-N-C catalyst was first synthesized by high-pressure pyrolysis in the presence of carbon support and thoroughly characterized in terms of morphology, structure and active site distribution. The subsequent electrochemical characterization of the catalyst shows strong adsorption and poisoning effect of, in addition to the known Cl⁻, perchloric anions on the oxygen reduction reaction (ORR) activity. On the contrary phosphate anions exhibit negligible poisoning effect on the catalyst activity. At 0.8V vs. RHE, the ORR activity of the catalyst is found to decrease in the order of H₃PO₄ (8.6mA mg⁻¹) > H₂SO₄ (5.3mA mg⁻¹) > HClO₄ (3.1mA mg⁻¹) > HCl (0.7mA mg⁻¹). The results suggest potential applications of NPMC in high-temperature PEMFCs based on phosphoric acid doped polymer membranes, where high loading platinum catalysts are currently used. As demonstrated in the low current density range of high-temperature PEMFCs, the catalyst shows a comparable performance to the Pt/C catalysts.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors
Authors: Hu, Y. (Intern), Jensen, J. O. (Intern), Pan, C. (Intern), Cleemann, L. N. (Intern), Shypunov, I. (Intern), Li, Q. (Intern)
Pages: 357-364
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information
Journal: Applied Catalysis B: Environmental
Impact of Polar Edge Terminations of the Transition Metal Dichalcogenide Monolayers during Vapor Growth

The polar edges of two-dimensional monolayer transition metal dichalcogenides (TMD) and their alloys are examined by combined theoretical (density functional theory) and experimental approaches. For these polar edges, the growth reaction energies between different edge terminations are considered instead of the surface free energies. Due to different energy evolutions during growth on the zigzag edges between MoS$_2$ and WS$_2$, the S-ZZ edges in the WS$_2$ monolayer flakes more easily decompose into sawtooth-like edges in M-ZZ type as compared to the MoS$_2$ monolayer; thus, the hexagonal morphology can be seen more often in WS$_2$. Moreover, the observed anisotropic short-range order in the MoS$_2$/WS$_2$ alloys is originated from the freezed edge configurations during growth, explainable by the growth kinetics and thermodynamics of the Mo-ZZ-edges. The determination of the growing edge terminations is of great importance for the controllable synthesis of the emergent two-dimensional TMD materials.
Influence of different technologies on dynamic pricing in district heating systems: Comparative case studies

District heating markets are often dominated by monopolies in both Denmark and Finland. The same companies, often owned by local municipalities, are usually operating both supplying plants and district heating networks, while the pricing mechanisms are rigid, often agreed upon for one year in advance. The mentioned ownership scheme may cause problems, when one tries to gain a third party access in order to deliver excess heat or heat from cheaper heating plants. In this paper, two case studies were carried out to simulate the district heating systems based on dynamic pricing. Case studies were carried out for Sønderborg, Denmark and Espoo, Finland. The results showed that dynamic pricing fosters feeding the waste heat into the grid, as dynamic pricing reduced the total primary energy consumption and CO₂ emissions in both case studies. In the best scenarios, the weighted average heat price decreased by 25.6% in Sønderborg and 6.6% in Espoo, respectively.

**General information**
- **State:** Published
- **Organisations:** Department of Energy Conversion and Storage, Centre for IT-Intelligent Energy Systems in Cities, Aalto University
- **Authors:** Dominkovic, D. F. (Intern), Wahlroos, M. (Ekstern), Syri, S. (Ekstern), Pedersen, A. S. (Intern)
- **Pages:** 136-148
- **Publication date:** 2018
- **Main Research Area:** Technical/natural sciences

**Publication information**
- **Journal:** Energy
- **Volume:** 153
- **ISSN (Print):** 0360-5442
- **Ratings:**
  - BFI (2018): BFI-level 2
  - Web of Science (2018): Indexed yes
  - BFI (2017): BFI-level 2
  - Scopus rating (2017): CiteScore 5.6 SJR 1.99 SNIP 1.923
  - Web of Science (2017): Indexed yes
  - BFI (2016): BFI-level 2
  - Scopus rating (2016): CiteScore 5.17 SJR 1.974 SNIP 1.823
  - Web of Science (2016): Indexed yes
  - BFI (2015): BFI-level 2
  - Scopus rating (2015): SJR 2.22 SNIP 2.037 CiteScore 5.03
  - Web of Science (2015): Indexed yes
Influence of iridium doping in MgB$_2$ superconducting wires

MgB$_2$ wires with iridium doping were manufactured using the in-situ technique in a composite Cu-Nb sheath. Reaction was performed at 700°C, 800°C or 900°C for 1h in argon atmosphere. A maximum of about 1.5 at.% Ir replaces Mg in MgB$_2$. The superconducting transition temperature is slightly lowered by Ir doping. The formation of IrMg$_3$ and IrMg$_4$ secondary phase particles is evidenced, especially for a nominal stoichiometry with 2.0 at.% Ir doping. The critical current density and accommodation field of the wires are strongly dependent on the Ir content and are generally weakened in the presence of Ir, although the effect is less pronounced at lower temperatures.
Influence of porosity on mechanical properties of tetragonal stabilized zirconia

3YSZ specimens with variable open porosity (1–57%) were fabricated, and the stiffness, strength and fracture properties (fracture toughness and R-curve) were measured to investigate their potential use as support structures for solid oxide fuel or electrolysis cells. The ball-on-ring test was used to characterize Young's modulus and Weibull strength. The variation of fracture toughness with porosity was investigated and modelled using the results from fracture mechanical testing. A distinct R-curve behaviour was observed in dense 3YSZ specimens, in samples with a porosity around 15% and in some of the highly porous samples (porosities ~45%) reflecting a transformation toughening in the material. For the most porous samples, the “R-curve behaviour” disappeared and subcritical crack growth was observed. The studies indicate that even highly porous 3YSZ structures (porosities exceeding 40%) are feasible supports for SOFC/SOECs from a mechanical point of view.
InGaN/GaN ultraviolet LED with a graphene/AZO transparent current spreading layer

We report an approach of using an interlayer of single layer graphene (SLG) for electroluminescence (EL) enhancement of an InGaN/GaN-based near-ultraviolet (NUV) light-emitting diode (LED) with an aluminum-doped zinc oxide (AZO)-based current spreading layer (CSL). AZO-based CSLs with and without a SLG interlayer were fabricated on the NUV LED epi-wafers. The current-voltage (I-V) characteristic and the EL intensity were measured and compared. We find that the LED without the SLG interlayer can possess a 40% larger series resistance. Furthermore, a 95% EL enhancement was achieved by the employment of the SLG interlayer.

General information
State: Published
Organizations: Department of Photonics Engineering, Diode Lasers and LED Systems, Department of Micro- and Nanotechnology, Optofluidics, Department of Energy Conversion and Storage, Electrochemical Materials and Interfaces, Nanoprobes, Center for Intelligent Drug Delivery and Sensing Using Microcontainers and Nanomechanics, DTU Danchip, Centre of Excellence for Silicon Photonics for Optical Communications, Chinese Academy of Sciences, Chinese Academy of Sciences
Authors: Lin, L. (Intern), Zhu, X. (Intern), Stamate, E. (Intern), Wu, K. (Intern), Liang, M. (Ekstern), Liu, Z. (Ekstern), Yi, X. (Ekstern), Herstrøm, B. (Intern), Boisen, A. (Intern), Jensen, F. (Intern), Ou, H. (Intern)
Number of pages: 9
Pages: 1818-1826
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information
Journal: Optical Materials Express
Volume: 8
Issue number: 7
ISSN (Print): 2159-3930
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
The reactions occurring at the oxygen electrodes of solid oxide fuel and electrolysis cells (SOFC/SOEC - SOC) were investigated, both with conventional techniques and with advanced in situ techniques, in order to study the reaction mechanisms and the surface evolution of the electrode materials under realistic operating temperatures and oxygen partial pressures. For this purpose, model (La,Sr)(Co,Fe)O3 (LSCF), (La,Sr)FeO3 (LSF) and La(Ni,Fe)O3 (LNF) electrodes were produced with pulsed laser deposition (PLD) and characterized using electrochemical impedance spectroscopy (EIS), X-ray photoelectron spectroscopy (XPS), scanning photoemission microscopy (SPEM) and high temperature scanning probe microscopy (SPM) with the additional functionality of Kelvin probe force microscopy (KPFM). In particular, XPS and SPEM represent novel tools with respect to solid state electrochemical characterization, as they have only recently been reaching relevant operating conditions in terms of obtainable temperatures and oxygen pressures in the experimental chambers.

KPFM is a less established technique with respect to SOC studies, being used mostly at low temperatures in corrosion science and for the study of semiconducting devices, but has a great potential and was optimized for the desired operating parameters during this work, obtaining promising results.

The influence of the experimental conditions on the surface exchange, as measured by EIS on model thin film electrodes produced by PLD, was the subject of the first main study. The influence of current constriction, current collector material and design and the purity of the gases proved to be most important with respect to Rsurf. However, other parameters were also evaluated, such as the stoichiometry of the thin films and their geometric area, but showed negligible effects with respect to the aforementioned parameters. The results succeeded in reproducing the scatter of three orders of magnitude present in literature data for the PLD, and resulted in a set of useful guidelines for measuring the intrinsic electrode materials performance and avoiding the influence of external artifacts.

In the second main study, the oxygen electrode reactions were studied under polarization, obtaining current-voltage profiles in varying oxygen partial pressures ranging between atmospheric oxygen content (210 mbar) and 10-1 mbar at 600 °C. These studies were integrated by surface chemistry characterization performed with XPS in an oxygen content between 1 mbar and 10-2 mbar at 600 °C, and with the added benefit of lateral spatial resolution of the surface chemistry with SPEM in 2.6-5×10-2 mbar oxygen at 600 °C. The surface chemistry characterization allowed an interpretation of the surface behavior, both in terms of degradation and with respect to the oxygen reactions, and for the first time a correlation between the electrode overpotential and the surface potential was deduced. Furthermore, the outcome of the studies of the electrode reactions under polarization also allowed the identification of the most probable reaction pathway for the oxygen incorporation.

SPEM was also used to investigate, with lateral spatial resolution, the surface chemistry and the electrical potential profiles in distributed electrodes deposited on thin electrolytes, in an attempt to contemporarily study the evolution of the surface chemistry and the distribution of the electric potentials in the LSCF electrodes and the GDC electrolyte under externally applied potential differences. The sample was designed as a model system which could replicate the composite nature of technological SOC electrodes. The overpotential distribution that was experimentally determined between the electrodes and the electrolyte was compared with finite element modelling simulations, showing good correspondence between the simulated values and the measured ones.

In order to approach the real operating conditions for the study of SOC materials, SPM and KPFM were performed in a specially designed microscope at temperatures of up to 600 °C in atmospheres ranging from pure N2 to pure O2 on a model sample, consisting of two isolated LNF electrodes on an MgO substrate. The sample could be used as a high temperature capacitor in order to evaluate the spatial resolution of KPFM in the relevant conditions, as well as the quality of the obtainable signal and the stability of commercial probes in more demanding operating conditions than the ones usually present in SPM setups. The results were very promising, and KPFM could represent a useful technique in future studies of SOC materials in realistic operating conditions, combining topographic characterization with chemical and...
We demonstrate an advanced approach using advanced in-situ transmission electron microscopy (TEM) to understand the interplay between nanostructures and thermoelectric (TE) properties of high-performance Mg-doped Zn4Sb3 TE system. With the technique, microstructure and crystal evolutions of TE material have been dynamically captured as a function of temperature from 300 K to 573 K. On heating, we have observed clearly precipitation and growth of a Zn-rich secondary phase as nanoinclusions in the matrix of primary Zn4Sb3 phase. Elemental mapping by STEM-EDX spectroscopy reveals enrichment of Zn in the secondary Zn6Sb5 nanoinclusions during the thermal processing without decomposition observed. Such nanostructure strongly enhances the phonon scattering resulting in the decrease in the thermal conductivity leading to a zT value of 1.4 at 718 K.
The EnovHeat project aims at developing an innovative heat pump system based on the magnetocaloric effect and active magnetic regenerator technology to provide for the heating needs of a single family house in Denmark. Unlike vapor-compression devices, magnetocaloric heat pumps use the reversible magnetocaloric effect of a solid refrigerant to build a cooling/heating cycle. It has the potential for high coefficient of performance, more silent operation and efficient part-load control. After presenting the operation principles of the magnetocaloric device and the different models used in the current numerical study, this article demonstrates for the first time the possibility to utilize this novel heat pump in a building. This device can be integrated in a single hydronic loop including a ground source heat exchanger and a radiant under-floor heating system. At maximum capacity, this magnetocaloric heat pump can deliver 2600 W of heating power with an appreciable average seasonal system COP of 3.93. On variable part-load operation with a simple fluid flow controller, it can heat up an entire house with an average seasonal system COP of 1.84.

**General information**

State: Published

Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, University of Southern Denmark, Aalborg Universitet København, Aalborg University
Intercalation of lithium into disordered graphite in a working battery

The structural transformations occurring during the intercalation of lithium into disordered graphite in a working battery were studied in detail by operando X-ray powder diffraction (XRPD). By using a capillary-based micro-battery cell, it was possible to study the stacking disorder in the initial graphite as well as in lithiated graphites. The micro-battery cell was assembled in its charged state with graphite as positive electrode and metallic lithium as counter electrode. The battery was discharged until a stage II compound (LiC12) was formed. The operando XRPD data reveal that the graphitic electrode material retains a disordered nature during the intercalation process. A DIFFaX+ refinement based on the initial operando XRPD pattern shows that the initial graphite generally has an intergrown structure with domains of graphite 2H and graphite 3R. However, the average stacking sequence of the initial graphite also contains a significant concentration of AA-type stacking of the graphene sheets. DIFFaX+ was further used to refine structure models of a stage III type compound and the final stage II compound. The refinement of the stage II compound showed that it is dominated by AαAαA-type stacking, but that it also contains a significant concentration of AαABβB-type slabs in the average stacking sequence.
Investigating particle size effects in catalysis by applying a size controlled and surfactant-free synthesis of colloidal nanoparticles in alkaline ethylene glycol - The case study of the oxygen reduction reaction on Pt

Colloidal platinum nanoparticles are obtained via a surfactant-free polyol process in alkaline ethylene glycol. In this popular synthesis, ethylene glycol functions as solvent and reducing agent. The preparation procedure is known for its reproducibility to obtain 1-2 nm nanoparticles, but at the same time the controlled preparation of larger nanoparticles is challenging. A reliable size control without the use of surfactants is a fundamental yet missing achievement for systematic investigations. In this work it is demonstrated how the molar ratio between NaOH and the platinum precursor determines the final particle size and how this knowledge can be used to prepare and study in a systematic way supported catalysts with defined size and metal loading. Using small-angle X-ray scattering, transmission electron microscopy, infra-red spectroscopy, X-ray absorption spectroscopy, pair distribution function and electrochemical analysis it is shown that changing the NaOH/Pt molar ratio from 25 to 3, the Pt nanoparticle size is tuned from 1 to 5 nm. This size range is of interest for various catalytic applications, such as the oxygen reduction reaction (ORR). Supporting the nanoparticles onto a high surface area carbon, we demonstrate how the particle size effect can be studied keeping the catalyst loading constant, an important aspect that in previous studies could not be accomplished.
Investment casting and experimental testing of heat sinks designed by topology optimization

Topology optimization (TO) is an attractive numerical tool to obtain optimized engineering designs, which has been originally developed for mechanical optimization and extended to the area of conjugate heat transfer. With rapid developments in topology optimization models, promising designs have been proposed and presented recently for conjugate heat transfer problems. However, only a very small number of experimental validations of TO heat transfer devices have been reported. In this paper, investment casting (IC) using 3D stereolithography (SLA) printed patterns is proposed to fabricate 3D metal heat transfer devices designed by TO. Three heat sinks for natural convection are designed by a previously reported topology optimization model and five reference pin-fin heat sinks are devised for comparison. From those designs six heat sinks are cast in Britannia metal, fully reproducing the complex 3D optimized designs. It shows that SLA-assisted IC is a very promising technology with low cost and high accuracy for fabricating TO metal parts, which is not limited to heat transfer devices and can be extended to other areas such as structural optimization. A natural convection experimental setup is used to experimentally study the performance of the fabricated heat sinks. The results show that the tested TO heat sinks can always realize the best heat dissipation performance compared to pin-fin heat sinks, when operating under the conditions used for the optimization. Moreover, validation simulations have been conducted to investigate the temperature distribution, fluid flow pattern and local heat transfer coefficient for the TO and pin-fin designs, further evidencing that TO designs always perform better under the design conditions. In addition, the impact of heat sink orientation and radiation are presented.
Joining of Half-Heusler and Bismuth Tellurides for Segmented Thermoelectric Generators

Segmented generators where the p- or n-type legs are formed by joining materials in series enables each material to operate in their most efficient temperature range. Here, we have fabricated and characterized segmented thermoelectric p- and n-type legs based on bismuth tellurides and half-Heusler alloys p-type Hf0.5Zr0.5CoSn0.2Sb0.8 and n-type Ti0.6Hf0.4NiSn. A two-step process was introduced to join the half-Heusler to the bismuth tellurides to form a segmented structure which was then characterized for its thermoelectric and structural properties. The output power generation was characterized under various hot side temperatures up to 873 K with the cold side fixed at 323 K. The stability of the joints was also investigated under heat treatment and thermal cycling. Under working temperatures from 323 K to 873 K, the obtained p-type segmented legs could deliver a power density of 0.3 W cm\(^{-2}\) and maximum voltage of 115 mV. With the same condition, the power density and the maximum voltage generated by n-type segmented leg were 0.25 W cm\(^{-2}\) and 102 mV. The area-specific contact resistances of the p- and n-type legs were 50 μΩ cm\(^2\) and 35 μΩ cm\(^2\), respectively. The output performance of each leg was âˆ¼ 95% after 6 cycles from 323 K to 873 K.
Water-based sol-gel electrospinning is employed to manufacture perovskite oxide \( \text{La}_{0.6}\text{Sr}_{0.4}\text{Co}_{0.2}\text{Fe}_{0.8}\text{O}_{3-\delta} \) (LSCF) nanofiber cathodes for intermediate-temperature solid oxide fuel cells. LSCF fibrous scaffolds are synthesized through electrospinning of a sol-gel solution employing water as the only solvent. Morphological characterizations demonstrate that the LSCF fibers have highly crystalline structure with uniform elemental distribution. After heat treatment, the average fiber diameter is 250 nm and the porosity of the nanofiber tissue is 37.5 %. The heat treated LSCF nanofibers are applied directly onto a \( \text{Ce}_{0.9}\text{Gd}_{0.1}\text{O}_{1.95} \) (CGO) electrolyte disk to form a symmetrical cell. Electrochemical characterization is carried out through electrochemical impedance spectroscopy (EIS) in the temperature range 550°C–950°C, and reproducibility of the electrochemical performance for a series of cells is demonstrated. At 650°C, the average measured polarization resistance \( R_p \) is 1.0 Ω cm². Measured performance decay is 1 % during the first 33h of operation at 750°C, followed by an additional 0.7 % over the subsequent 70h.
LCA of Energy Systems

Energy systems are essential in the support of modern societies’ activities, and can span a wide spectrum of electricity and heat generation systems and cooling systems. Along with their central role and large diversity, these systems have been demonstrated to cause serious impacts on human health, ecosystems and natural resources. Over the past two decades, energy systems have thus been the focus of more than 1000 LCA studies, with the aim to identify and reduce these impacts. This chapter addresses LCA applications to energy systems for generation of electricity and heat. The chapter gives insight into the LCA practice related to such systems, offering a critical review of (i) central methodological aspects, including the definition of the goals and scopes of the studies, their coverage of the system life cycle and the environmental impacts, and (ii) key findings of the studies, particularly aimed at identifying environmental hotspots and impact patterns across different energy sources. Based on this literature review recommendations and guidelines are issued to LCA practitioners on key methodological aspects that are important for a proper conduct of LCA studies of energy systems and thus ensuring the reliability of the LCA results provided to decision- and policy-makers.

General information
State: Published
Organisations: Transport DTU, Department of Management Engineering, Quantitative Sustainability Assessment, Department of Energy Conversion and Storage
Authors: Laurent, A. (Intern), Espinosa Martinez, N. (Intern), Hauschild, M. Z. (Intern)
Pages: 633-668
Publication date: 2018

Host publication information
Title of host publication: Life Cycle Assessment: Theory and practice
Publisher: Springer
ISBN (Print): 9783319564746
Chapter: 26
Main Research Area: Technical/natural sciences
Life Cycle Assessment of Hydrogen Production and Consumption in an Isolated Territory

Hydrogen produced from renewables works as an energy carrier and as energy storage medium and thus hydrogen can help to overcome the intermittency of typical renewable energy sources. However, there is no comprehensive environmental performance study of hydrogen production and consumption. In this study, detailed cradle to grave life cycle analyses are performed in an isolated territory. The hydrogen is produced on-site by Polymer Electrolyte Membrane (PEM) water electrolysis based on electricity from wind turbines that would otherwise have been curtailed and subsequently transported with gas cylinder by road and ferry. The hydrogen is used to provide electricity and heat through fuel cell stacks as well as hydrogen fuel for fuel cell vehicles. In order to evaluate the environmental impacts related to the hydrogen production and utilisation, this work conducts an investigation of the entire life cycle of the described hydrogen production, transportation, and utilisation. All the processes related to the equipment manufacture, operation, maintenance, and disposal are considered in this study.

Lithium Conductivity and Ions Dynamics in LiBH4/SiO2 Solid-Electrolytes studied by Solid-State NMR and Quasi Elastic Neutron Scattering and applied in Lithium-Sulfur Batteries

Composite solid-state electrolytes based on ball-milled LiBH4/SiO2 aerogel exhibit high lithium conductivities and we have found an optimal weight ratio, 30/70 wt% LiBH4/SiO2, with a conductivity of 0.1 mS/cm-1 at room temperature. We have studied the Li+ and BH4- dynamics using Quasi- Elastic Neutron Scattering and solid-state Nuclear Magnetic Resonance and found that only a small fraction (~10%) of the ions have high mobilities while most of the LiBH4 shows behavior similar to macrocrystalline material. The modified LiBH4 is formed from interaction with the SiO2 surface and most probably from reaction with the surface silanol groups. We successfully applied these composite electrolytes in lithium-sulfur solid-state batteries. The batteries show reasonable capacity retention (794 mAhg-1 sulfur after 10 discharge-charge cycles, coulombic efficiency of 88.8% ± 2.7% and average capacity loss of 7.2% during the first 10 cycles)
Localized carbon deposition in solid oxide electrolysis cells studied by multiphysics modeling

Solid oxide electrochemical cells (SOCs) can store electrical energy in the form of chemical fuels with high efficiency by electrolysis of CO₂ and H₂. However, achieving commercially relevant lifetime is hindered by degradation mechanisms such as carbon deposition, which can even destroy the cell especially during electrolysis where carbon formation is electrochemically driven at the electrode-electrolyte interface. Here we used a three-dimensional multiphysics model to simulate a SOC performing CO₂ electrolysis and determine the operating conditions and locations in the porous nickel-based electrodes where carbon deposition is expected based on local conditions (gas composition, temperature and overpotential) crossing local thermodynamic thresholds. It is found that CO/CO₂ gas diffusion gradients and cooling from the endothermic electrolysis reaction are important driving forces for carbon deposition to occur locally when it is not expected based on the outlet CO concentration. Furthermore, correlation with a set of experimentally determined threshold operating points indicates that carbon deposition occurs primarily by the Boudouard reaction rather than by direct electrochemical reduction of CO or CO₂ to carbon for the studied cell type. Variation of fuel electrode porosity and thickness shows that these methods of reducing gas diffusion limitations widen the operating window that avoids carbon deposition.
Long-Term Durability of PBI-Based HT-PEM Fuel Cells: Effect of Operating Parameters

This work studies the long-term durability of high-temperature polymer electrolyte membrane fuel cells based on acid-doped polybenzimidazole membranes. The primary focus is on acid loss via the evaporation mechanism, which is a major cause of degradation in applications that involve long-term operation. Durability is assessed for 16 identically fabricated membrane electrode assemblies (MEAs), and evaluations are carried out using operating parameters as stressors with gas stoichiometries ranging from 2 to 25, current densities from 200 to 800 mA cm\(^{-2}\), and temperatures of 160 or 180 degrees C. Cell diagnostics are composed of time resolved polarization curves, post mortem analysis, and in situ temperature measurements. A major part of the cell degradation during these steady-state tests can be ascribed to increasing area-specific series resistance. By means of post mortem acid-loss measurements, the degradation is correlated to the temperature and to the accumulated gas-flow volume. Such relations are indicative of acid loss via evaporation. Current density also plays a critical role for the acid loss and, thus, for the overall cell degradation. The effect of current is likely tied to mechanisms that involve water generation, migration of electrolyte ions, and locally elevated temperature inside the MEAs. (C) The Author(s) 2018. Published by ECS.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors, Danish Power Systems Ltd.
Authors: Søndergaard, T. (Intern), Cleemann, L. N. (Intern), Becker, H. (Intern), Steenberg, T. (Ekstern), Hjuler, H. A. (Ekstern), Seerup, L. (Intern), Li, Q. (Intern), Jensen, J. O. (Intern)
Pages: F3053-F3062
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of the Electrochemical Society
Volume: 165
Issue number: 6
ISSN (Print): 0013-4651
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 3.48 SJR 1.267 SNIP 1.009
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.97 SJR 1.222 SNIP 0.963
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.115 SNIP 1.066 CiteScore 3.17
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.213 SNIP 1.25 CiteScore 3.36
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.169 SNIP 1.309 CiteScore 2.92
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.329 SNIP 1.281 CiteScore 2.61
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.331 SNIP 1.335 CiteScore 2.74
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.418 SNIP 1.304
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.442 SNIP 1.27
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.595 SNIP 1.41
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.569 SNIP 1.322
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.608 SNIP 1.535
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.523 SNIP 1.481
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.712 SNIP 1.7
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.971 SNIP 1.677
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 2.036 SNIP 1.618
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 1.663 SNIP 1.729
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 1.632 SNIP 1.7
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 1.6 SNIP 1.846

Original language: English
Machine learning-based screening of complex molecules for polymer solar cells

Polymer solar cells admit numerous potential advantages including low energy payback time and scalable high-speed manufacturing, but the power conversion efficiency is currently lower than for their inorganic counterparts. In a Phenyl-C_{61}-Butyric-Acid-Methyl-Ester (PCBM)-based blended polymer solar cell, the optical gap of the polymer and the energetic alignment of the lowest unoccupied molecular orbital (LUMO) of the polymer and the PCBM are crucial for the device efficiency. Searching for new and better materials for polymer solar cells is a computationally costly affair using density functional theory (DFT) calculations. In this work, we propose a screening procedure using a simple string representation for a promising class of donor-acceptor polymers in conjunction with a grammar variational autoencoder. The model is trained on a dataset of 3989 monomers obtained from DFT calculations and is able to predict LUMO and the lowest optical transition energy for unseen molecules with mean absolute errors of 43 and 74 meV, respectively, without knowledge of the atomic positions. We demonstrate the merit of the model for generating new molecules with the desired LUMO and optical gap energies which increases the chance of finding suitable polymers by more than a factor of five in comparison to the randomised search used in gathering the training set.
Magnetoelastic phase diagram of TbNi$_2$B$_2$C

The magnetic phase diagram of the quaternary borocarbide TbNi$_2$B$_2$C is investigated by direct means and by studying magnetically induced modifications of the crystal structure. Detailed Superconducting quantum interference device measurements reveal a complex phase diagram with five distinct magnetic phases. The phase boundaries are mapped out comprehensively. Synchrotron hard x-ray measurements in applied magnetic fields are employed to probe the magnetoelastic distortions throughout the phase diagram. The determination of the wave vectors of these field-induced lattice deformations suggests a range of commensurate spin-slip-type magnetic structures at low temperatures with wave vectors of the form $(q,0,0)$ with $q = 6/11$ and $5/9$. The proposed magnetic structures yield values of magnetization well in-line with observations. The scattering intensity due to the magnetoelastic deformations exhibits a drastic jump at the phase boundary at 1.3 T and low temperatures.

General information

State: Published

Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Department of Energy Conversion and Storage, Electrofunctional materials, Department of Wind Energy, Wind Turbine Structures and Component Design, Technical University of Denmark, University of Copenhagen, Deutsches Elektronen-Synchrotron, Helmholtz–Zentrum Berlin für Materialien und Energie, Ochanomizu University, National Institute for Materials Science

Mechanical stability of roll-to-roll printed solar cells under cyclic bending and torsion

The ability of printed organic solar cells (OSCs) to survive repeated mechanical deformation is critical to large-scale implementation. This paper reports an investigation into the mechanical stability of OSCs through bending and torsion testing of whole printed modules. Two types of modules are used that differ slightly in thickness as well as on the basis of the electrode materials: silver nanowires or carbon-based inks. Each type of module is subjected to two different mechanical modes of deformation, bending and torsion, of several thousand cycles per module using a purpose-built robotic device. Analysis of the distribution of stress in the devices performed by finite-element modeling predicts the locations of failure. Failure upon bending originates at the laser-cut edges of the modules from shear at the clamp/module interface leading to crazing of the plastic barrier encapsulant foils. This crazing leads to eventual delamination due first to decohesion of the active layer at the edge of the modules and later to deadhesion between the PEDOT:PSS (electrode) and P3HT:PCBM (semiconductor) layers. The torsion mode imposes greater stresses than the bending mode and thus leads to failure at fewer strain cycles. Failure during torsion occurs through crack propagation initiated at stress concentrations on the edges of the module that were imposed by their rectangular geometry and ultimately leads to bifurcation of the entire module. Rather than the differences in electrode materials, the differences in survivability between the two types of modules are attributed mostly to the thickness of the substrate materials used, with the thinner substrate used in the carbon-based modules (~160 Åm) failing at fewer strain cycles than the substrate used in the silver-nanowire-based modules (~190 Åm). Taken together, the results suggest ways in which the lifetimes of devices can be extended by the layouts of modules and choices of materials.
Organic solar cell, Conjugated polymer, Flexible electronics, Barrier encapsulation, Mechanical stability, Cyclic fatigue testing

DOIs: 10.1016/j.solmat.2017.08.015
Source: FindIt
Source-ID: 2373352207
Publication: Research - peer-review › Journal article – Annual report year: 2018

Melting behaviour of raw materials and recycled stone wool waste
Stone wool is a widely used material for building insulation, to provide thermal comfort along with fire stability and acoustic comfort for all types of buildings. Stone wool waste generated either during production or during renovation or demolition of buildings can be recycled back into the stone wool melt production. This study investigates and compares the thermal response and melting behaviour of a conventional stone wool charge and stone wool waste. The study combines differential scanning calorimetry (DSC), hot stage microscopy (HSM) and X-ray diffraction (XRD). DSC reveals that the conventional charge and stone wool waste have fundamentally different thermal responses, where the charge experiences gas release, phase transition and melting of the individual raw materials. The stone wool waste experiences glass transition, crystallization and finally melting. Both DSC and HSM measurements indicates that the wool waste initiates melting at a lower temperature than the conventional charge. Also DSC measurements show that the wool waste requires less energy for heating and melting than the conventional charge, making stone wool waste recycling desirable both for environmental and for process purposes.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, Department of Energy Conversion and Storage, Mixed Conductors, Rockwool International
Authors: Schultz-Falk, V. (Intern), Agersted, K. (Ekstern), Jensen, P. A. (Intern), Solvang, M. (Ekstern)
Pages: 34-41
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Non-Crystalline Solids
Volume: 485
ISSN (Print): 0022-3093
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 1.19 SJR 0.722 CiteScore 2.42
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.02 SJR 0.685 SNIP 1.167
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.663 SNIP 1.079 CiteScore 1.85
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.794 SNIP 1.182 CiteScore 1.87
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.813 SNIP 1.174 CiteScore 1.79
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.755 SNIP 1.108 CiteScore 1.64
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.844 SNIP 1.268 CiteScore 1.7
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.91 SNIP 1.112
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.922 SNIP 0.992
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.956 SNIP 1.207
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.947 SNIP 1.081
Scopus rating (2006): SJR 0.911 SNIP 1.158
Scopus rating (2005): SJR 1.003 SNIP 1.144
Scopus rating (2004): SJR 1.007 SNIP 1.209
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.427 SNIP 1.341
Scopus rating (2002): SJR 0.809 SNIP 1.144
Scopus rating (2001): SJR 1.215 SNIP 1.154
Scopus rating (2000): SJR 1.141 SNIP 1.11
Scopus rating (1999): SJR 1.027 SNIP 0.963
Original language: English
Stone wool, Melting, Waste, Recycling
DOIs:
https://doi.org/10.1016/j.jnoncrysol.2018.01.035
Source: Bibtex
Source-ID: urn:205788c766ed221e417e7b451d4a4fa1
Publication: Research - peer-review › Journal article – Annual report year: 2018
MgO as a non-pyrolyzable pore former in porous membrane supports
The gas permeability of Y0.03Zr0.97O2 (3Y-TZP) porous supports from thermoplastic feedstocks has been improved by adding MgO as a non-pyrolyzable pore former. Common pyrolyzable pore formers such as graphite often produce tortuous and narrow pore channels with low gas permeability, limiting the performance of oxygen transport membranes or other membranes relying on gas transport to the active membrane surface. Thermoplastic feedstocks for extrusion of tubular 3Y-TZP supports were prepared with four different amounts of pyrolyzable pore formers and/or MgO as non-pyrolyzable pore former. The MgO was removed after sintering by leaching in acetic acid. With this technique we obtained porosities above 70 vol% and gas permeabilities above 3 10-14 m2. Compared to samples with only pyrolyzable pore formers, the non-pyrolyzable pore former increases the gas permeability and reduces the tortuosity.
Modelling smart energy systems in tropical regions

A large majority of energy systems models of smart urban energy systems are modelling moderate climate with seasonal variations, such as the European ones. The climate in the tropical region is dominated by very high stable temperatures and high humidity and lacks the moderate climate's seasonality. Furthermore, the smart energy system models tend to focus on CO₂ emissions only and lack integrated air pollution modelling of other air pollutants. In this study, an integrated urban energy system for a tropical climate was modelled, including modelling the interactions between power, cooling, gas, mobility and water desalination sectors. Five different large scale storages were modelled, too. The developed linear optimization model further included endogenous decisions about the share of district versus individual cooling, implementation of energy efficiency solutions and implementation of demand response measures in buildings and industry. Six scenarios for the year 2030 were developed in order to present a stepwise increase in energy system integration in a transition to a smart urban energy system in Singapore. The economically best performing scenario had 48% lower socio-economic costs, 68% lower CO₂e emissions, 15% higher particulate matter emissions and 2% larger primary energy consumption compared to a business-as-usual case.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Energy Systems Analysis, Department of Management Engineering, Systems Analysis, Centre for IT-Intelligent Energy Systems in Cities, Wageningen University & Research,
Nanoscale patterning of electronic devices at the amorphous LaAlO3/SrTiO3 oxide interface using an electron sensitive polymer mask

A simple approach is presented for designing complex oxide mesoscopic electronic devices based on the conducting interfaces of room temperature grown LaAlO3/SrTiO3 heterostructures. The technique is based entirely on methods known from conventional semiconductor processing technology, and we demonstrate a lateral resolution of similar to 100 nm. We study the low temperature transport properties of nanoscale wires and demonstrate the feasibility of the technique for defining in-plane gates allowing local control of the electrostatic environment in mesoscopic devices. (C) 2018 Author(s).

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, University of Copenhagen, Technical University of Denmark
Number of pages: 5
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information
Volume: 112
Issue number: 17
Article number: 171606
ISSN (Print): 0003-6951
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 3.25 SJR 1.382 SNIP 1.167
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.67 SJR 1.673 SNIP 1.249
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.499 SNIP 1.226 CiteScore 2.47
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.861 SNIP 1.492 CiteScore 3.25
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.146 SNIP 1.633 CiteScore 3.77
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 2.57 SNIP 1.739 CiteScore 3.76
ISI indexed (2012): ISI indexed yes
In this study, the origin of noise in electrochemical impedance spectroscopy (EIS) spectra measured on a variety of polymer electrolyte membrane electrolysis cells (PEMECs) has been investigated. EIS was measured during operation at various current densities of seven different PEMECs divided in five different cell types including both acidic PEMECs and alkaline PEMECs. The noise pattern differed between various types of cells and between cells of the same cell type. Integration time had no influence on the EIS noise level, whereas the AC amplitude seems to influence the EIS noise level. Other electrical noise sources influencing the EIS measurements have been studied with oscilloscope. No noise was observed at DC. A hypothesis explaining the relation between bubble formation during electrolysis and EIS noise is proposed based on the experimental findings.
EIS, EIS noise, Electrochemical Impedance Spectroscopy, Gas Bubbles, Nafion 117, PEMEC, Polymer Electrolyte Membrane Electrolysis Cell

DOI: 10.1002/fuce.201800005
Non-enzymatic glucose sensing platform using self assembled cobalt oxide/graphene nanocomposites immobilized graphite modified electrode

A new strategy to prepare the densely packed cobalt oxide (Co3O4)/graphene nanocomposites by a self-assembly method were adopted in this work. A new non-enzymatic glucose determination has been fabricated by using Co3O4/graphene nanocomposites modified electrode as a sensing material. The nanocomposites were characterized using X-ray diffraction, X-ray photoelectron spectroscopy and field emission scanning electron microscopy, which confirms the successful formation of dense packed Co3O4/graphene nanocomposite. The results of Co3O4/graphene nanocomposites modified electrode exhibit good electrocatalytic activity toward the oxidation of glucose in 0.1 M NaOH by cyclic voltammetry. Under optimal conditions, the oxidation peak current was proportional to the glucose concentration in the range from 16.0 μM to 1.3 mM with a detection limit of 0.5 μM. The determination of glucose with the modified electrode shows the advantages of ease of preparation, high sensitivity and good stability. The analytical utility of the modified electrode as an amperometric sensor for the determination of glucose in the flow systems was evaluated by chronoamperometric studies. The practical application of the modified electrode for glucose determination has been evaluated in urine samples.
Nucleation front instability in two-dimensional (2D) nanosheet gadolinium-doped cerium oxide (CGO) formation

Herein we report for the first time the synthesis of ceramic–organic three-dimensional (3D) layered gadolinium-doped cerium oxide (Ce$_{1-x}$Gd$_x$O$_{2-x}$, CGO) and its exfoliation into two-dimensional (2D) nanosheets. We adopt a water-based synthetic route via homogenous precipitation approach at low temperatures (10–80 °C). The reaction conditions are tuned to investigate the effects of thermal energy on the final morphology. A low temperature (40 °C) morphological transition from nanoparticles (1D) to two-dimensional (2D) nanosheets is observed and associated with a low thermal energy transition of ca. 2.6 kJ mol$^{-1}$. For the 3D-layered material, exfoliation experiments are conducted in water/ethanol solutions. Systems at volume fractions ranging from 0.15 to 0.35 are demonstrated to promote under ultrasonic treatment the delamination into 2D nanosheets.

General information

State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Imaging and Structural Analysis, Electrofunctional materials, Nuclear and Energy Research Institute, Universidade Federal do ABC
Authors: Marani, D. (Intern), Moraes, L. P. R. (Ekstern), Gualandris, F. (Intern), Sanna, S. (Intern), Zanetti De Florio, D. (Ekstern), Esposito, V. (Intern), Fonseca, F. C. (Ekstern)
Pages: 1405-1410
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information

Journal: CrystEngComm
Volume: 20
Issue number: 10
ISSN (Print): 1466-8033
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 0.823 SJR 0.998 CiteScore 3.25
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.37 SJR 1.053 SNIP 0.904
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.04 SNIP 0.987 CiteScore 3.83
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Numerical simulation of kinetic demixing and decomposition in a LaCoO$_{3-\delta}$ oxygen membrane under an oxygen potential gradient

A composition- and temperature-dependent mobility database of all ionic species in the LaCoO$_{3-\delta}$ phase was developed and combined with a La-Co-O thermodynamic database to simulate kinetic demixing and partial decomposition in LaCoO$_{3-\delta}$ oxygen membranes operated under a 0.0001/0.21 bar oxygen partial pressure difference at 1073 K for 1 year. Formation of La$_2$O$_3$, Co$_3$O$_4$ and CoO phases across the membrane is predicted. The kinetic demixing process can be divided into two stages, namely, establishment of the oxygen potential gradient (fast) and demixing of the cations (slow); the former is controlled by the mobility of oxygen ions, and the latter is determined by the higher mobility of Co ions as compared to the La ion in the ABO$_3$-type perovskite. A drift motion of both oxide surfaces towards the high P$_{O2}$ side occurs with the movement of cations.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Central South University
Pages: 526-539
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information
Operation Strategies Based on Carbon Corrosion and Lifetime Investigations for High Temperature Polymer Electrolyte Membrane Fuel Cell Stacks

This paper is aimed to develop operation strategies or high temperature polymer electrolyte fuel cells (HT-PEMFCs) stacks in order to enhance the endurance by mitigating carbon oxidation reaction. The testing protocols are carefully designed to suit the operating cycle for the realistic application. A 5 cell co-flow stack is assembled with BASF Celtec® P membrane electrode assembly (MEA) with an active area of 163.5 cm². The oxidation rate of carbon is systematically investigated employing potentiostatic experiments under variation of both cell voltage and temperature using on-line mass spectrometry. The experimental results show that more CO2 is measured for the open circuit voltage (OCV) operation, indicating that the lifetime of the stack is strongly affected by a factor of approximately 12–26 between OCV and 700 mV depending on temperature. Protective start-stop algorithms are developed to avoid the formation of aggressive cell potentials. The startup procedures let degrade the catalyst support to a higher extent than the stop procedures, which is presumably due to both OCV exposure and hydrogen front passing through the anode. A model for lifetime prediction is developed from carbon corrosion experiments and validated with a durability test for 1,562 cycle events.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Zentrum für Sonnenenergie- und Wasserstoff-Forschung Baden-Württemberg
Authors: Kannan, A. (Intern), Kaczerowski, J. (Ekstern), Kabza, A. (Ekstern), Scholta, J. (Ekstern)
Pages: 287-298
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information
Journal: Fuel Cells
Volume: 18
Issue number: 3
ISSN (Print): 1615-6846
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 1.88 SJR 0.559 SNIP 0.748
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.79 SJR 0.495 SNIP 0.603
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.685 SNIP 0.779 CiteScore 2.02
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.615 SNIP 0.792 CiteScore 2.05
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.835 SNIP 0.833 CiteScore 1.99
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.24 SNIP 0.993 CiteScore 2.76
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.639 SNIP 1.247 CiteScore 3.31
ISI indexed (2011): ISI indexed yes
In this work, we investigated the long-term oxidation behavior of a Ni-Fe (1:1 weight ratio) support for solid oxide fuel cell (SOFC) applications. Ni-Fe supports were obtained through tape casting, high temperature sintering and pre-reducing in 97% H₂/N₂ (9/91)-3% H₂O at 750 and 1000°C, respectively. Then the Ni-Fe supports were exposed in simulated anode atmospheres of 97% H₂/N₂ (9/91)-3% H₂O and 75% H₂/N₂ (9/91)-25% H₂O for periods of up to 1000h at 750°C. The samples were examined for mass change, phase and chemical composition, and microstructure evolution during the annealing process. The Ni-Fe supports exposed to H₂/N₂-3% H₂O showed negligible oxidation, while those exposed to H₂/N₂-25% H₂O showed a 4-6% mass increase, due to the fact that a Fe-rich oxide scale was found on the surface of the Ni-Fe alloy particles. Room-temperature conductivity measurements showed that the supports annealed in the two atmospheres maintained sufficiently high conductivity. The results from the current work demonstrate that the porous Ni-Fe support can be well employed in SOFCs, especially metal-supported SOFCs.
Oxidation of Ethylene Carbonate on Li Metal Oxide Surfaces

Understanding the reactivity of the cathode surface is of key importance to the development of batteries. Here, density functional theory is applied to investigate the oxidative decomposition of the electrolyte component, ethylene carbonate (EC), on layered LiMO$_2$ oxide surfaces. We compare adsorption energy trends of atoms and small molecules, on both surface oxygen and metal sites, as a function of the Li content of the surface. The oxygen sites are identified as the reactive site for the electrolyte oxidation reaction (EOR). We report reaction energies and NEB-calculated kinetic barriers for the initial oxidative decomposition of EC, and correlate both with the reaction energy of hydrogen adsorption on oxygen. The hydrogen adsorption energy scales with the distance between the Fermi level and the O-2p band center. We
expect this model of the EOR to be valid for other organic electrolytes and other Li metal oxide surfaces, due to its simplicity, and the model leads to simple design principles for protective coatings.
Oxide Modules

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Ceramic Engineering & Science
Authors: Le, T. H. (Intern), Van Nong, N. (Intern), Pryds, N. (Intern)
Pages: 719-734
Publication date: 2018

Host publication information
Title of host publication: Advanced Thermoelectrics: Materials, Contacts, Devices, and Systems
Publisher: CRC Press
ISBN (Print): 9781498765725
Chapter: 21
Main Research Area: Technical/natural sciences
Source: PublicationPreSubmission
Source-ID: 134385072
Publication: Research › Book chapter – Annual report year: 2018

Oxygen Exchange and Transport in (La0.6Sr0.4)0.98FeO3-d– Ce0.9Gd0.1O1.95 Dual-Phase Composites
The chemical diffusion coefficient and the effective surface exchange coefficient (kex) of dual-phase (La0.6Sr0.4)0.98FeO3-d (LSF) – Ce0.9Gd0.1O1.95 (CGO) composites containing between 30 and 70 vol.% of CGO were determined by electrical conductivity relaxation (ECR) at high oxygen partial pressures (10⁻³ < pO₂ < 1 atm) and at temperatures between 600°C and 900°C. The surface impurity segregation was detected by TOF-SIMS analysis. A large enhancement of kex was observed with increasing CGO fraction in the composite. kex was increased from 3.51 × 10⁻⁵ cm/s for a pure LSF to 1.86 × 10⁻⁴ cm/s for a 70 vol.% of CGO in the composite at 750°C for a pO₂ change from 0.2 to 1.0 atm. The experiments demonstrate that the kex is enhanced due to a synergistic effect between the two phases, and suggest a direct involvement of CGO phase in the oxygen surface exchange reaction. Possible mechanisms that could account for the synergy are the oxygen exchange process occurs also on the CGO surface, for example a spillover of absorbed oxygen ions from the LSF surface to the CGO surface or scavenging of impurities from one phase to another, thereby improving the oxygen exchange properties of the cleaned phase.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors
Authors: Ovtar, S. (Intern), Søgaard, M. (Intern), Norrman, K. (Intern), Hendriksen, P. V. (Intern)
Pages: F220-F231
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of the Electrochemical Society
Volume: 165
Issue number: 3
ISSN (Print): 0013-4651
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Performance and stability of (ZrO$_{2.89}$Y$_{0.01}$Sc$_{0.10}$LaCr$_{0.85}$Cu$_{0.10}$Ni$_{0.05}$O$_{3-\delta}$ oxygen transport membranes under conditions relevant for oxy-fuel combustion

Self-standing, planar dual-phase oxygen transport membranes consisting of 70 vol.% (ZrO$_2$)$_{0.89}$(Y$_2$O$_3$)$_{0.01}$(Sc$_2$O$_3$)$_{0.10}$ (10Sc1YSZ) and 30 vol.% LaCr$_{0.85}$Cu$_{0.10}$Ni$_{0.05}$O$_{3-\delta}$ (LCCN) were successfully developed and tested. The stability of the composite membrane was studied in simulated oxy-fuel power plant flue-gas conditions (CO$_2$, SO$_2$, H$_2$O). The analyses of the exposed composites by X-ray diffraction (XRD), X-ray fluorescence (XRF), attenuated total reflection Fourier transform infrared spectroscopy (ATR-FTIR) and Raman spectroscopy revealed an excellent stability. Oxygen permeation fluxes were measured across 1000 $\mu$m thick and 110 $\mu$m thick self-supported 10Sc1YSZ-LCCN (70-30 vol.%) membranes from 700 °C to 950 °C using air as the feed gas and N$_2$ or CO$_2$ as the sweep gas. The 110 $\mu$m thick membrane, prepared by tape-casting and lamination processes, showed oxygen fluxes up to 1.02 mLN cm$^{-2}$ min$^{-1}$ (950 °C, air/N2). Both membranes demonstrated stable performances over long-term stability tests (250-300 h) performed at 850 °C using pure CO$_2$ as the sweep gas.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Ceramic Engineering & Science, Korea Institute of Energy Research, Imperial College London
Pages: 115-123
Publication date: 2018
Main Research Area: Technical/natural sciences
Plasma and catalyst for the oxidation of NOx

Efficient exhaust gas cleaning from NOx (NO and NO2) by absorption and adsorption based methods requires the oxidation of NO. The application of non-thermal plasma is considered as a promising oxidation method but the oxidation of NO by direct plasma remains limited due to the back-reaction of NO2 to NO mediated by O radicals in plasma. Indirect NO oxidation by plasma produced ozone allows to circumvent the back-reaction and further oxidize NO2 to N2O5 but the slow reaction rate for the latter process limits the efficiency of this process. Present paper gives an overview of the role of metal-oxide catalysts in the improvement of oxidation efficiency for both direct and indirect plasma oxidation of NOx. The plasma produced active oxygen species (O, O3) were shown to play an important role in the reactions taking place on the catalyst surfaces while the exact mechanism and extent of the effect were different for direct and indirect oxidation. In the case of direct plasma oxidation, both short and long lifetime oxygen species could reach the catalyst and participate in the oxidation of NO to NO2. The back-reaction in the plasma phase remained still important factor and limited the effect of catalyst. In the case of indirect oxidation, only ozone could reach the catalyst surface and improve the oxidation of NO2 to N2O5. The effect of catalyst at different experimental conditions was quantitatively described with the aid of simple global chemical kinetic models derived for the NOx oxidation either by plasma or ozone. The models allowed to compare the effect of different catalysts and to analyze the limitations for the efficiency improvement by catalyst.

General information

State: Published
Organisations: Department of Energy Conversion and Storage, University of Tartu
Authors: Jõgi, I. (Ekstern), Erme, K. (Ekstern), Levoll, E. (Ekstern), Raud, J. (Ekstern), Stamate, E. (Intern)
Number of pages: 14
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information
Journal: Plasma Sources Science and Technology
Volume: 27
Issue number: 3
Article number: 035001
ISSN (Print): 0963-0252
Ratings:
BFI (2018): BFI-level 1
P-type Al-doped Cr-deficient CrN thin films for thermoelectrics

Thermoelectric properties of chromium nitride (CrN)-based films grown on c-plane sapphire by dc reactive magnetron sputtering were investigated. In this work, aluminum doping was introduced in CrN (degenerate n-type semiconductor) by co-deposition. Under the present deposition conditions, over-stoichiometry in nitrogen (CrN$_{1+\delta}$) rock-salt structure is obtained. A p-type conduction is observed with nitrogen-rich CrN combined with aluminum doping. The Cr$_{0.96}$Al$_{0.04}$N$_{1.17}$ film exhibited a high Seebeck coefficient and a sufficient power factor at 300 °C. These results are a starting point for designing p-type/n-type thermoelectric materials based on chromium nitride films, which are cheap and routinely grown on the industrial scale.
Quantum heat engines: Limit cycles and exceptional points

We show that the inability of a quantum Otto cycle to reach a limit cycle is connected with the propagator of the cycle being noncompact. For a working fluid consisting of quantum harmonic oscillators, the transition point in parameter space where this instability occurs is associated with a non-Hermitian degeneracy (exceptional point) of the eigenvalues of the propagator. In particular, a third-order exceptional point is observed at the transition from the region where the eigenvalues are complex numbers to the region where all the eigenvalues are real. Within this region we find another exceptional point, this time of second order, at which the trajectory becomes divergent. The onset of the divergent behavior corresponds to the modulus of one of the eigenvalues becoming larger than one. The physical origin of this phenomenon is that the hot and cold heat baths are unable to dissipate the frictional internal heat generated in the adiabatic strokes of the cycle. This behavior is contrasted with that of quantum spins as working fluid which have a compact Hamiltonian and thus no exceptional points. All arguments are rigorously proved in terms of the systems’ associated Lie algebras.
Reactivating the Ni-YSZ electrode in solid oxide cells and stacks by infiltration

The solid oxide cell (SOC) could play a vital role in energy storage when the share of intermittent electricity production is high. However, large-scale commercialization of the technology is still hindered by the limited lifetime. Here, we address this issue by examining the potential for repairing various failure and degradation mechanisms occurring in the fuel electrode, thereby extending the potential lifetime of a SOC system. We successfully infiltrated the nickel and yttria-stabilized zirconia cermet electrode in commercial cells with Gd-doped ceria after operation. By this method we fully reactivated the fuel electrode after simulated reactant starvation and after carbon formation. Furthermore, by infiltrating after 900h of operation, the degradation of the fuel electrode was reduced by a factor of two over the course of 2300h. Lastly, the scalability of the concept is demonstrated by reactivating an 8-cell stack based on a commercial design.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry
Authors: Skafte, T. L. (Intern), Hjelm, J. (Intern), Blennow Tullmar, P. (Intern), Graves, C. R. (Intern)
Pages: 685-690
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Power Sources
Volume: 378
ISSN (Print): 0378-7753
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 7 SJR 2.202 SNIP 1.536
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 6.22 SJR 1.944 SNIP 1.5
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Re-activation of degraded nickel cermet anodes - Nano-particle formation via reverse current pulses

The Ni/yttria-stabilized-zirconia (YSZ) cermet is the most commonly applied fuel electrode for solid oxide cells (SOCs). Loss of Ni/YSZ electrode activity is a key life-time limiting factor of the SOC. Developing means to mitigate this loss of performance or re-activate a fuel electrode is therefore important.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry, Politecnico di Torino
Authors: Hauch, A. (Intern), Marchese, M. (Ekstern), Lanzini, A. (Ekstern), Graves, C. R. (Intern)
Pages: 110-120
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Power Sources
Volume: 377
ISSN (Print): 0378-7753
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 7 SJR 2.202 SNIP 1.536
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 6.22 SJR 1.944 SNIP 1.5
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.9 SNIP 1.667 CiteScore 6.34
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.964 SNIP 2.042 CiteScore 6.3
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.975 SNIP 2.137 CiteScore 5.63
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.282 SNIP 2.006 CiteScore 5.04
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.227 SNIP 2.172 CiteScore 5.13
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 2.294 SNIP 1.972
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 2.105 SNIP 1.785
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.96 SNIP 1.713
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.587 SNIP 1.488
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.802 SNIP 2.223
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.656 SNIP 1.809
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.85 SNIP 1.805
Scopus rating (2003): SJR 1.66 SNIP 1.57
Scopus rating (2002): SJR 2.385 SNIP 1.409
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 1.146 SNIP 1.506
Scopus rating (2000): SJR 0.649 SNIP 0.949
Reassignment of 'magic numbers' for Au clusters of decahedral and FCC structural motifs
Calculations of low free energy structures of gold clusters with a few hundred to a few thousand atoms have been performed. For the study to be computationally feasible, a systematic scheme for generating low energy atomic structures with a given structural motif and a chosen size is used. Comparison of the relative stability of clusters with the decahedral and FCC motifs reveals periodic windows of stability for asymmetric, open-shell FCC clusters while the stability of the decahedral structural motif shows a smoother variation in stability with cluster size. As a result, the FCC structural motif is most stable for clusters with around 440, 610, 800, 1050... atoms, while the decahedral motif is more stable for atomic numbers of around 525, 705, 925, 1175... These new 'magic numbers' represent regions around which a number of asymmetric, open shell clusters of a given motif are most stable, in contrast to the discrete set of highly symmetric magic size structures that are commonly cited. As temperature is raised, the decahedral motif gains stability over the FCC motif. These results help explain reported experimental observations and can guide future laboratory preparations of shape selected clusters.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, University of Otago, ETH Zurich
Authors: Garden, A. L. (Ekstern), Pedersen, A. (Ekstern), Jonsson, H. (Intern)
Pages: 5124-5132
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information
Journal: Nanoscale
Volume: 10
Issue number: 11
ISSN (Print): 2040-3364
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 7.57 SJR 2.934 SNIP 1.442
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 7.46 SJR 2.789 SNIP 1.441
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 2.77 SNIP 1.542 CiteScore 7.97
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.646 SNIP 1.649 CiteScore 7.64
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.558 SNIP 1.467 CiteScore 6.89
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 2.769 SNIP 1.349 CiteScore 6.08
ISI indexed (2012): ISI indexed yes
Sample Design and Preparation Techniques for Dynamic Microstructural Studies of High Temperature Electrochemical Cells

Understanding the dynamics of 3D microstructural change in high temperature electrochemical cells, primarily solid oxide fuel cells or electrolyzers, is a pressing driving force for performing time resolved ex-situ, in-situ and in-operando nano-tomography and diffraction based experiments at synchrotron X-ray sources. These experiments must meet simultaneous challenging demands: precision beamline compatible samples that are stable at high temperature, supply of electric potential, and control of atmosphere. Correct sample design is an absolute necessity for experimental success. Here, the merits of possible sample configurations and environments are explored and evaluated against fabrication challenges and experimental feasibility. Experience with designing and performing experiments of selected configurations will be presented. Results of 3D nano-tomography of Ni-yttria stabilized zirconia (YSZ) fuel electrode microstructure evolution during Ni oxidation, reduction and annealing, and spatially resolved in-operando diffraction studies of YSZ electrolytes under high polarization will be summarised.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Imaging and Structural Analysis, Neutrons and X-rays for Materials Physics, Department of Physics, Paul Scherrer Institut, ESRF-The European Synchrotron
Authors: Bowen, J. R. (Intern), De Angelis, S. (Intern), Sierra Trujillo, J. X. (Intern), Jørgensen, P. S. (Intern), Poulsen, H. F. (Intern), Hsiao Rho Tsai, E. (Ekstern), Holler, M. (Ekstern), Villanova, J. (Ekstern), Cook, P. (Ekstern)
Number of pages: 1
Publication date: 2018
Event: Abstract from 4th International Congress on 3D Materials Science (3DMS 2018), Helsingør, Denmark.
Main Research Area: Technical/natural sciences
Electronic versions:
3DMS_2018_Bowen_JR_Sample_design_for_dynamic_high_temperature_electrochemical_cell_microstructure_studies.pdf
Links:
http://www.programmaster.org/PM/PM.nsf/ViewSessionSheets?OpenAgent&amp;ParentUNID=48D8FB4F739C65BA8525827B0050ACBA
Source: PublicationPreSubmission
Source-ID: 149880778
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2018

Scaling up aqueous processing of A-site deficient strontium titanate for SOFC anode supports

All ceramic anode supported half cells of technically relevant scale were fabricated in this study, using a novel strontium titanate anode material. The use of this material would be highly advantageous in solid oxide fuel cells due to its redox tolerance and resistance to coking and sulphur poisoning. Successful fabrication was possible through aqueous tape casting of both anode support and electrolyte layers and subsequent lamination. Screen printing of electrolyte layers onto green anode tapes was also attempted but resulted in cracked electrolyte layers upon firing. Microstructural, electrical and mechanical properties of anode supports and half cells will be discussed. The use of two different commercial titanate powders with nominal identical, but in reality different stoichiometries, strongly affect electrical and mechanical properties. Careful consideration of such variations between powder suppliers, and batches of the same supplier, is critical for the successful implementation of ceramic anode supported solid oxide fuel cells.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, University of St Andrews, Forschungszentrum Jülich GmbH
Authors: Verbraeken, M. C. (Ekstern), Sudireddy, B. R. (Intern), Vasechko, V. (Ekstern), Cassidy, M. (Ekstern), Ramos, T. (Intern), Malzbender, J. (Ekstern), Holtappels, P. (Intern), Irvine, J. T. (Ekstern)
Sintering of MnCo2O4 coatings prepared by electrophoretic deposition

Sintering of MnCo2O4 coatings prepared by electrophoretic deposition on steel substrates has been studied in air and in reducing-oxidizing atmosphere. Effect of temperature and pO2 on the resulting coating density was evaluated from scanning electron microscopy images of polished cross sections. Best sample microstructure defined by having high density and no cracks, was found after a reduction at 1000 °C and reoxidation at 900 °C.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, AGH University of Science and Technology
Authors: Bobruk, M. (Ekstern), Molin, S. (Intern), Chen, M. (Intern), Brylewski, T. (Ekstern), Hendriksen, P. V. (Intern)
Number of pages: 5
Pages: 394-398
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information
Journal: Materials Letters
Volume: 213
ISSN (Print): 0167-577X
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SJR 0.782 SNIP 0.887 CiteScore 2.68
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.51 SJR 0.754 SNIP 0.939
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.767 SNIP 0.993 CiteScore 2.5
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.877 SNIP 1.28 CiteScore 2.64
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.824 SNIP 1.221 CiteScore 2.41
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.917 SNIP 1.383 CiteScore 2.41
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.014 SNIP 1.546 CiteScore 2.54
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.056 SNIP 1.276
Sliding-wear resistance of pure near fully-dense B₄C under lubrication with water, diesel fuel, and paraffin oil

The sliding-wear resistance of pure near fully-dense B₄C is investigated, and the wear mode/mechanisms identified, under lubrication with water, diesel fuel, and paraffin oil. It is found that the wear is mild in the three cases, with specific wear rates (SWRs) of 10⁻¹⁶–10⁻¹⁷ m³/N m. Nonetheless, the wear resistance of the B₄C ceramic is one order of magnitude greater under oil lubrication (10⁻¹⁶ N m/m²) than under water lubrication (10⁻¹⁵ N m/m²), and twice as great for the specific case of paraffin oil than diesel fuel, attributable to the lubricant’s viscosity. It is also found that the wear mode is always abrasion, and that the wear mechanisms are plastic deformation and localized fracture with grain pullout. However, in agreement with the macro-wear data, the severity of the wear damage is lower under lubrication with paraffin oil, followed by diesel fuel, and lastly water. Finally, microstructural considerations are discussed with a view to enhancing the sliding-wear resistance of B₄C triboceramics.
Smart nano-inks for inkjet printing of functional oxide based thin films

The development of thin oxide based films for energy production and storage has been in the center of attention for the past decades. Performances of film based devices, such as solar cells, solid oxide fuel cells (SOFC), or sensors is strongly linked to the thickness of the active layers, with thinner layers often providing enhanced performances. The success in the development and usability of such energy production devices is linked to the deposition technique chosen for the layer fabrication. The technique should be reproducible, industrially scalable and low cost to be viable as well as commercially attractive. Among thin film fabrication processes, inkjet printing is a high potential candidate.

Inkjet printing is a deposition method based on the jetting of very small droplets (approx. 10-12 l) onto substrates. It is a mask-less, non-contact additive patterning technique that allows the deposition of complex patterns with high positional accuracy of the droplets (typically in the micron-range spacing) with high speed and low cost. Due to these features, this processing method shows a strong potential as a thin film fabrication method. For the past decades inkjet printing of functional materials has been developed and studied as an alternative to spin coating, lithography, etching or physical vapor deposition technique such as pulse laser deposition (PLD) for the fabrication of metal oxide based thin films. One
critical aspect in inkjet printing is the ink design and its long term stability. Instability can lead to undesirable nozzle clogging and unresolved printing that lower the global performance of the device.

This thesis presents the development and characterization of three inks designs which differs by the oxide source: a suspension of colloidal particles, a solution metallic precursor-based particle free ink, and a combination of both solution and suspension, here called hybrid ink. The major goal of this work was to evaluate the printability and the stability potentials of different ink designs for inkjet printing, and the pros/cons of each of them. The ink printability and stability is particularly evaluated through rheology, chemical characterization and droplet jetting observation. Films made of some relevant functional ceramics such as zirconium-, cerium- and titanium-oxide based materials are successfully fabricated with printers using different droplet ejection principles to demonstrate the versatility of the inks. Microstructure and performance of the films after heat treatment is characterized and show enhanced performance compared to films processed with different methods.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science
Authors: Gadea, C. (Intern)
Number of pages: 235
Publication date: 2018

Publication information
Place of publication: Kgs. Lyngby
Publisher: Technical University of Denmark (DTU)
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
Thesis_Final_version_for_print_JT.pdf

Relations
Projects:
Smart nano-inks for inkjet printing of functional oxide based thin films
Publication: Research › Ph.D. thesis – Annual report year: 2018

Stoichiometric control in Bi$_4$Ti$_3$O$_{12}$ synthesis by novel hybrid solid state reaction
The synthesis of bismuth titanate Bi$_4$Ti$_3$O$_{12}$(BiT) is performed via a novel solid state reaction. The reaction is designed to control the stoichiometric content of the highly volatile element, i.e. Bi. The chemical route consists in trapping bismuth oxide colloids in a stabilized titanium based sol gel solution. The resulting colloidal-solution hybrid ink can be processed via various ceramic processes. After gelation of TiO$_2$ in the sol-gel component the mixture reacts at high temperature (850°C) to yield the BiT phase. The obtained material is c-axis oriented, and its lattice parameters, shrinkage and density matches the pure Bi$_4$Ti$_3$O$_{12}$ phase. The sintered material exhibits enhanced higher dielectric constant (232) than usually reported for this phase.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Electrofunctional materials, Silpakorn University
Authors: Gadea, C. (Intern), Phatharapeetranun, N. (Ekstern), Ksapabutr, B. (Ekstern), Grivel, J. (Intern), Esposito, V. (Intern)
Pages: 101-103
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information
Journal: Materials Letters
Volume: 221
ISSN (Print): 0167-577X
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SJR 0.782 SNIP 0.887 CiteScore 2.68
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.51 SJR 0.754 SNIP 0.939
Structural and superconducting characteristics of YBa$_2$Cu$_3$O$_7$ films grown by fluorine-free metal-organic deposition route

Microstructure and superconducting performance of YBa$_2$Cu$_3$O$_7$ (YBCO) films deposited on LaAlO$_3$ single crystal (LAO) substrates by a fluorine-free metal-organic deposition (FF-MOD) technique, have been studied by means of X-ray reciprocal space mapping (RSM), cross-sectional transmission electron microscopy (TEM) and magnetooptical (MO) imaging. Combining the X-ray diffraction and the TEM cross-sectional analysis, it is revealed that stacking faults, i.e. YBa$_2$Cu$_4$O$_{x}$ intergrowths, and ab-plane twins are main defects in the FF-MOD YBCO films. Due to the highly epitaxial growth mechanism related to transient liquid phase, the LAO twinned substrate structure is also inherited in the FF-YBCO films. The low-density planar defects containing dislocations parallel to c-axis result in stripy patterns observed in the MO images. For comparison, the low-fluorine (LF) MOD film show a texture mosaic spread in the ab plane and is little influenced by the LAO twinning underneath, implying the severe structural disorder most likely associated with the large amount of small-angle grain boundaries. Moreover, the higher density of stacking faults was also detected by XRD 0-2θ, scan in the LF-MOD film. It is suggested that associated partial dislocations formed at the boundary between the
stacking faults and YBCO matrix act as strong linear (or dot) pinning centers. These structural characteristics are well in line with the better superconducting performance of the low fluorine-MOD film, in particular under external magnetic field at 77 K. This work offers an in-depth insight into the correlation between the microstructure and superconductivity in the MOD YBCO films.

**General information**

State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Shanghai Jiao Tong University, University of Oslo
Authors: Zhao, Y. (Ekstern), Chu, J. (Ekstern), Qureishy, T. (Ekstern), Wu, W. (Ekstern), Zhang, Z. (Ekstern), Mikheenko, P. (Ekstern), Johansen, T. H. (Ekstern), Grivel, J. (Intern)
Pages: 844-852
Publication date: 2018
Main Research Area: Technical/natural sciences

**Publication information**

Journal: Acta Materialia
Volume: 144
ISSN (Print): 1359-6454
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 6.18 SJR 3.263 SNIP 2.737
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 5.67 SJR 3.21 SNIP 2.702
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 3.417 SNIP 2.831 CiteScore 5.22
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 3.885 SNIP 3.166 CiteScore 5.16
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 3.238 SNIP 2.674 CiteScore 4.37
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 3.37 SNIP 2.875 CiteScore 4.28
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 3.215 SNIP 2.768 CiteScore 4.27
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 3.709 SNIP 2.698
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 3.663 SNIP 2.625
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 3.82 SNIP 2.774
Web of Science (2008): Indexed yes
Web of Science (2007): Indexed yes
Studies of A-site Deficient (Gd$_{0.6}$Sr$_{0.4}$)$_{1–x}$Fe$_{0.8}$Co$_{0.2}$O$_{3–x}$ Cathodes in SOFCs

A series of A-site deficient Gd-containing Fe-Co-based cathodes were synthesized using the glycine-nitrate process. All the compounds consisted of two phases, i.e., a cubic and orthorhombic phase, as determined by powder X-ray diffraction (XRD). The thermal expansion coefficient decreased with increasing A-site deficiency, which could be because cobalt was expelled from the main phases. Likewise, the electrochemical activities of the Gd-containing Fe-Co-based solid oxide fuel cell cathodes toward the reduction of oxygen were improved by a factor of approximately 3 by making them A-site deficient. The composition (Gd$_{0.6}$Sr$_{0.4}$)$_{0.85}$Fe$_{0.8}$Co$_{0.2}$O$_{3–x}$ showed the highest activity toward the reduction of oxygen among the five compounds. Electrochemical impedance spectroscopy estimated the area specific resistance as 5.77 Ω cm$^2$ at 600 °C. The electrochemical impedance spectroscopy measurements revealed three arcs for most of the compounds at the three temperatures where the measurements were performed.
Subsolidus phase equilibria of the CuO–SrO–ZnO pseudoternary system in air at 900 °C

The subsolidus phase equilibria of the CuO–SrO–ZnO system were determined at 900 °C in air. The pseudoternary section does not contain ternary oxide phases but is made of 5 three-phase regions and 2 narrow two-phase regions linked to a Sr\textsubscript{14}Cu\textsubscript{24−x}Zn\textsubscript{x}O\textsubscript{41−y} solid solution. The maximum solubility of Zn in this phase is limited to x≈ 0.1, but this low doping level results in a significant decrease of the electrical resistivity by about one order of magnitude compared to the undoped compound. The other binary oxide phases SrZnO\textsubscript{2}, Sr\textsubscript{2}CuO\textsubscript{3}, and SrCuO\textsubscript{2} do not form solid solutions extending into the ternary system. SrZnO\textsubscript{2} was found to decompose upon contact with ambient air.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Authors: Grivel, J. (Intern)
Pages: 6-15
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information
Journal: Chimica Techno Acta
Graphitic layer encapsulated iron based nanoparticles (G@FeNPs) have recently been disclosed as an interesting type of highly active electrocatalysts for the oxygen reduction reaction (ORR). However, the complex composition of the metal-containing components and their contributions in catalysis remain unclear. As a representative catalyst of the unique encapsulated structure, a series of G@FeNPs catalysts were prepared by a high-pressure pyrolytic process with uniform and essentially identical morphologies but varied compositions. The catalysts exhibited a high onset potential of 0.85 V at 0.1 mA cm\(^{-2}\) in acidic media. By \(^{57}\)Fe-Mössbauer spectroscopy the iron containing components were identified including α-Fe, γ-Fe, γ-Fe\(_2\)O\(_3\), and Fe\(_3\)C as well as a minor doublet component due to Fe\(^{3+}\) in high spin and/or Fe\(^{2+}\) in low spin state. The ORR activities are evaluated in terms of the mass specific kinetic current density found to be positively correlated with the Fe\(_3\)C content in the range of study, indicating involvement of the encapsulated nanoparticles in the ORR catalysis. The recognition of the Fe compositions and active sites provides new insights to the confined Fe-based ORR electrocatalysts and therefore options for further development of non-precious metal materials.
Synthesis and stability of strongly acidic benzamide derivatives

Reactivity studies of strong organic acids based on the replacement of one or both of the oxygens in benzoic acids with the trifluoromethanesulfonamide group are reported. Novel derivatives of these types of acids were synthesized in good yields. The generated N-triflylbenzamides were further functionalized through cross-coupling and nucleophilic aromatic substitution reactions. All compounds were stable in dilute aqueous solutions. Studies of stability under acidic and basic conditions are also reported.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors, University of Copenhagen
Authors: Diness, F. (Ekstern), Bjerrum, N. J. (Intern), Begtrup, M. (Ekstern), O'Hagan, D. (ed.) (Ekstern)
Pages: 523-530
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information
Volume: 14
ISSN (Print): 2195-951X
Ratings:
BFI (2018): BFI-level 1
Synthesis and thermal decomposition study of dysprosium trifluoroacetate

A study of the thermal decomposition process of dysprosium trifluoroacetate hydrate under flowing argon is presented. Thermogravimetry, differential thermal analysis, evolved gas analysis and ex-situ x-ray diffraction techniques have been employed in the investigation. Three main stages were identified: dehydration, decomposition and phase transformation from DyF$_3$ to DyFO. The dehydration takes place in 2 steps and the decomposition also occurs in two stages. The observed residual mass demonstrated a discrepancy with the calculated value for DyF$_3$ formation. Observations on quenched samples at temperatures just above the decomposition step and at 828°C showed a variation in the sample color, being dark in the first case and rather bright at the higher quenching temperature. Based on this fact, we concluded that some carbon remains in the sample up to 800°C. With the temperature reaching 1300°C, a plateau is observed in the TG signal, which mass value agrees with the formation of DyFO as verified by the ex-situ x-ray data of quenched powder. Using the FTIR and MS spectra of released gases during the process and the TG data, a decomposition scheme is suggested.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Authors: Opata, Y. A. (Intern), Grivel, J. (Intern)
Pages: 40-46
Publication date: 2018
Main Research Area: Technical/natural sciences
The Impact of Strong Cathodic Polarization on Ni|YSZ Microelectrodes

This work is a study of the impact of short-term strong cathodic polarization in a Ni|YSZ model system using Ni probes as working microelectrodes in a high temperature scanning probe microscope at 650°C in humidified 9% H₂ in N₂. Impedance spectroscopy revealed one to three orders of magnitude decrease in the high frequency resistance and four to
A five orders of magnitude decrease in the low frequency impedance with polarization from $-1.06 \text{ V to } -3.06 \text{ V vs E}^\circ(\text{O}_2)$, indicating introduction of electronic conductivity and expansion of the reaction zone around the Ni microelectrode. The effect on the Ni|YSZ interface included formation of electronic conductance, reaction between Ni and YSZ and accumulation of impurities around the Ni|YSZ contact as verified by conductance scans of the polarized area. Cyclic voltammetry was used to compare three systems with different impurity levels and showed that the presence of silicates reduces the current, i.e. lowers the performance of the electrode reaction.

**General information**

State: Published
Organisations: Department of Energy Conversion and Storage, Department of Chemistry
Authors: Kreka, K. (Intern), Hansen, K. V. (Intern), Mogensen, M. B. (Intern), Norman, K. (Intern), Chatzichristodoulou, C. (Intern), Jacobsen, T. (Intern)
Pages: F253-F263
Publication date: 2018
Main Research Area: Technical/natural sciences

**Publication information**

Journal: Journal of the Electrochemical Society
Volume: 165
Issue number: 5
ISSN (Print): 0013-4651
Ratings:

- BFI (2018): BFI-level 1
- Web of Science (2018): Indexed yes
- BFI (2017): BFI-level 1
- Scopus rating (2017): CiteScore 3.48 SJR 1.267 SNIP 1.009
- Web of Science (2017): Indexed yes
- BFI (2016): BFI-level 1
- Scopus rating (2016): CiteScore 2.97 SJR 1.222 SNIP 0.963
- Web of Science (2016): Indexed yes
- BFI (2015): BFI-level 1
- Scopus rating (2015): SJR 1.115 SNIP 1.066 CiteScore 3.17
- Web of Science (2015): Indexed yes
- BFI (2014): BFI-level 1
- Scopus rating (2014): SJR 1.213 SNIP 1.25 CiteScore 3.36
- Web of Science (2014): Indexed yes
- BFI (2013): BFI-level 1
- Scopus rating (2013): SJR 1.169 SNIP 1.309 CiteScore 2.92
- ISI indexed (2013): ISI indexed yes
- Web of Science (2013): Indexed yes
- BFI (2012): BFI-level 1
- Scopus rating (2012): SJR 1.329 SNIP 1.281 CiteScore 2.61
- ISI indexed (2012): ISI indexed yes
- Web of Science (2012): Indexed yes
- BFI (2011): BFI-level 1
- Scopus rating (2011): SJR 1.331 SNIP 1.335 CiteScore 2.74
- ISI indexed (2011): ISI indexed yes
- Web of Science (2011): Indexed yes
- BFI (2010): BFI-level 1
- Scopus rating (2010): SJR 1.418 SNIP 1.304
- Web of Science (2010): Indexed yes
- BFI (2009): BFI-level 1
- Scopus rating (2009): SJR 1.442 SNIP 1.27
- Web of Science (2009): Indexed yes
- BFI (2008): BFI-level 1
- Scopus rating (2008): SJR 1.595 SNIP 1.41
- Web of Science (2008): Indexed yes
Thermochemical stability of zirconia-titanium nitride as mixed ionic-electronic composites

Dense zirconia (8% molar yttria-stabilized ZrO2)-titanium nitride (TiN) composites are fabricated to obtain mixed ionic-electronic conducting ceramic systems with high degree of electronic and thermal conductivity. The composites are consolidated by spark plasma sintering (SPS), starting from pure powders of the pristine phases mixed in different ratios (TiN = 25, 50, 75 wt%). A careful optimization of the SPS conditions allows producing highly dense samples with no reaction between the phases or degradation by oxidation, thus maintaining the chemical integrity of the two phases. For all the composites, high electrical conductivity is attained. Samples exhibit metallic behavior, showing an unexpected percolation of TiN in the YSZ matrix for volume fraction ≤ 25 wt% (27 vol%). Chemical degradation and electrical properties of the compounds were monitored under oxidative (air) and inert (Ar) atmosphere at high temperatures. The oxidation kinetics of the nitride phase was inhibited by the microstructure of the composite. The electrical properties of such composites were explored at high temperature to evaluate its application in electrochemical devices. As results, it is shown that electrical transport properties of the composite can be tuned by both the relative volume fraction of phases and controlled oxidative treatments. Adjusting such parameters different electric behaviors were observed ranging from predominant electronic conductors, to temperature-independent resistivity, and semiconducting.
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 2.85 SJR 0.784 SNIP 1.167
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.88 SJR 0.844 SNIP 1.376
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.823 SNIP 1.281 CiteScore 2.64
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.856 SNIP 1.645 CiteScore 2.76
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.799 SNIP 1.552 CiteScore 2.28
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.81 SNIP 1.736 CiteScore 2.08
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.918 SNIP 1.733 CiteScore 2.1
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.855 SNIP 1.292
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.932 SNIP 1.468
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.866 SNIP 1.639
Scopus rating (2007): SJR 0.902 SNIP 1.417
Scopus rating (2006): SJR 0.809 SNIP 1.216
Scopus rating (2005): SJR 0.522 SNIP 0.993
Scopus rating (2004): SJR 0.681 SNIP 1.454
Scopus rating (2003): SJR 0.701 SNIP 0.997
Scopus rating (2002): SJR 0.66 SNIP 0.886
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.548 SNIP 0.881
Scopus rating (2000): SJR 0.46 SNIP 0.787
Scopus rating (1999): SJR 0.496 SNIP 0.796
Original language: English
Yttria-stabilized zirconia, TiN, Composite, Spark plasma sintering, Mixed ionic-electronic conductors
DOIs:
10.1016/j.ceramint.2018.02.039
Source: FindIt
Source-ID: 2396397813
Publication: Research - peer-review › Journal article – Annual report year: 2018
The Role of Pore-Formers on Grain Interior and Grain Boundary Conductivity in Tape-Cast Porous Sheets for Electrochemical Flue Gas Purification

$\text{Ce}_{0.9}\text{Gd}_{0.1}\text{O}_{1.95}$ (CGO) electrolytes for electrochemical flue gas purification were fabricated by means of tape casting with different types, shapes and sizes of pore-formers. The sintered bodies were characterized with electrochemical impedance spectroscopy, to investigate the role of the different pore-formers on the electrochemical properties of the cast tapes. A strong effect of the different pore-formers on the conductivity (both grain interior and grain boundary conductivities) was observed. In addition, the conductivity data were also correlated with previously obtained gas permeability data. The conductivity data correlated with the permeability data in the sense that a higher permeability lead to a lower conductivity. The porosity of the samples also influenced the conductivities. The higher the porosity of the sintered bodies, the lower the conductivity was, as expected.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science
Authors: Schmidt, C. G. (Intern), Andersen, K. B. (Intern), Stamate, E. (Intern), Kaiser, A. (Intern), Kammer Hansen, K. (Intern)
Pages: 485-492
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Ceramic Science and Technology
Volume: 8
Issue number: 4
ISSN (Print): 2190-9385
Ratings:
Web of Science (2018): Indexed yes
Scopus rating (2017): CiteScore 1.4
Scopus rating (2016): CiteScore 1.13
Scopus rating (2015): CiteScore 0.53
Scopus rating (2014): CiteScore 0.62
Scopus rating (2013): CiteScore 0.5
Scopus rating (2012): CiteScore 0.98
Original language: English
CGO, Tape casting, EIS, Conductivity
DOIs:
10.4416/JCST2017-00024
Source: PublicationPreSubmission
Source-ID: 142691347
Publication: Research - peer-review › Journal article – Annual report year: 2018

Three dimensional characterization of nickel coarsening in solid oxide cells via ex-situ ptychographic nano-tomography
Nickel coarsening is considered a significant cause of solid oxide cell (SOC) performance degradation. Therefore, understanding the morphological changes in the nickel-yttria stabilized zirconia (Ni-YSZ) fuel electrode is crucial for the wide spread usage of SOC technology. This paper reports a study of the initial 3D microstructure evolution of a SOC analyzed in the pristine state and after 3 and 8 h of annealing at 850 °C, in dry hydrogen. The analysis of the evolution of the same location of the electrode shows a substantial change of the nickel and pore network during the first 3 h of treatment, while only negligible changes are observed after 8 h. The nickel coarsening results in loss of connectivity in the nickel network, reduced nickel specific surface area and decreased total triple phase boundary density. For the condition of this experiment, nickel coarsening is shown to be predominantly curvature driven, and changes in the electrode microstructure parameters are discussed in terms of local microstructural evolution.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Imaging and Structural Analysis, Paul Scherrer Institut
Authors: De Angelis, S. (Intern), Jørgensen, P. S. (Intern), Tsai, E. H. R. (Ekstern), Holler, M. (Ekstern), Kreka, K. (Intern), Bowen, J. R. (Intern)
Pages: 72-79
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Power Sources
Volume: 383
ISSN (Print): 0378-7753
Ratings:

BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 7 SJR 2.202 SNIP 1.536
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 6.22 SJR 1.944 SNIP 1.5
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.9 SNIP 1.667 CiteScore 6.34
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.964 SNIP 2.042 CiteScore 6.3
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.975 SNIP 2.137 CiteScore 5.63
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.282 SNIP 2.006 CiteScore 5.04
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.227 SNIP 2.172 CiteScore 5.13
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 2.294 SNIP 1.972
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 2.105 SNIP 1.785
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.96 SNIP 1.713
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.587 SNIP 1.488
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.802 SNIP 2.223
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.656 SNIP 1.809
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.85 SNIP 1.805
Scopus rating (2003): SJR 1.66 SNIP 1.57
Scopus rating (2002): SJR 2.385 SNIP 1.409
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 1.146 SNIP 1.506
Scopus rating (2000): SJR 0.649 SNIP 0.949
Scopus rating (1999): SJR 0.814 SNIP 0.988
Original language: Undefined/Unknown
Nano-tomography, Solid oxide cell, Nickel coarsening, Ex-situ, Ptychography
DOI's: 10.1016/j.jpowsour.2018.02.031
Three Dimensional Polarimetric Neutron Tomography of Magnetic Fields

Through the use of Time-of-Flight Three Dimensional Polarimetric Neutron Tomography (ToF 3DPNT) we have for the first time successfully demonstrated a technique capable of measuring and reconstructing three dimensional magnetic field strengths and directions unobtrusively and non-destructively with the potential to probe the interior of bulk samples which is not amenable otherwise. Using a pioneering polarimetric set-up for ToF neutron instrumentation in combination with a newly developed tailored reconstruction algorithm, the magnetic field generated by a current carrying solenoid has been measured and reconstructed, thereby providing the proof-of-principle of a technique able to reveal hitherto unobtainable information on the magnetic fields in the bulk of materials and devices, due to a high degree of penetration into many materials, including metals, and the sensitivity of neutron polarisation to magnetic fields. The technique puts the potential of the ToF time structure of pulsed neutron sources to full use in order to optimise the recorded information quality and reduce measurement time.
This paper investigates the application of density-based topology optimization to the design of air-cooled forced convection heat sinks. To reduce the computational burden that is associated with a full 3D optimization, a pseudo 3D optimization model comprising a 2D modeled conducting metal base layer and a thermally coupled 2D modeled thermofluid design layer is used. Symmetry conditions perpendicular to the flow direction are applied to generate periodic heat sink designs. The optimization objective is to minimize the heat sink heat transfer resistance for a fixed pressure drop over the heat sink and a fixed heat production rate in the base plate. Optimized designs are presented and the resulting fin geometry is discussed from a thermal engineering point of view and compared to fin shapes resulting from a pressure drop minimization objective. Parametric studies are conducted to analyze the influence of the pressure drop on the heat sink heat transfer resistance. To quantify the influence of the assumptions made in the pseudo 3D optimization model, validation simulations with a body-fitted mesh in 2D and 3D are conducted. A good agreement between optimization model and validation simulations is found, confirming the physical validity of the utilized optimization model. Two topology optimized designs are exemplarily benchmarked against a size optimized parallel fin heat sink and an up to 13.6% lower thermal resistance is found to be realized by the topology optimization.
Towards High Power Density Metal Supported Solid Oxide Fuel Cell for Mobile Applications

For use of metal supported solid oxide fuel cell (MS-SOFC) in mobile applications it is important to reduce the thermal mass to enable fast startup, increase stack power density in terms of weight and volume and reduce costs. In the present study, we report on the effect of reducing the Technical University of Denmark (DTU) SoA MS-SOFCs support layer thickness from 313 μm gradually to 108 μm. The support layer thickness decrease in the DTU co-sintering MS-SOFC fabrication route results in an increased densification of the support layer and a slight decrease in performance. To mitigate the performance loss, two different routes for increasing the porosity of the support layer and thus performance were explored. The first route is the introduction of gas channels by puncturing of the green tape casted support layer. The second route is modification of the co-sintering profile. In summary, the cell thickness and thus weight and volume was reduced and the cell power density at 0.7 V at 700°C was increased by 46% to 1.01 W/cm−2 at a fuel utilization of 48%. All modifications were performed on a stack technological relevant cell size of 12 cm × 12 cm.
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 3.48 SJR 1.267 SNIP 1.009
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.97 SJR 1.222 SNIP 0.963
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.115 SNIP 1.066 CiteScore 3.17
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.213 SNIP 1.25 CiteScore 3.36
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.169 SNIP 1.309 CiteScore 2.92
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.329 SNIP 1.281 CiteScore 2.61
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.331 SNIP 1.335 CiteScore 2.74
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.418 SNIP 1.304
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.442 SNIP 1.27
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.595 SNIP 1.41
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.569 SNIP 1.322
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.608 SNIP 1.535
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.523 SNIP 1.481
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.712 SNIP 1.7
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.971 SNIP 1.677
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 2.036 SNIP 1.618
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 1.663 SNIP 1.729
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 1.632 SNIP 1.7
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 1.6 SNIP 1.846

Original language: English
Towards solar cells with black silicon texturing passivated by a-Si:H

We introduce surfaces of black silicon (bSi) fabricated by reactive ion etch (RIE) and passivated by hydrogenated amorphous silicon (a-Si:H). We demonstrate minority effective lifetime over 1.5 ms for the best bSi surfaces, corresponding to over 700 mV of implied open circuit voltage, values higher than on reference surfaces prepared by KOH etching. Fabrication of solar cells resulted in promising efficiency of 16.1 % for bSi as compared to 18.5 % for KOH references. Quantum efficiency measurements revealed that the bSi cells lose approximately 0.5 mA cm⁻² in the visible and 0.8-1 mA cm⁻² in the infrared (IR) region. Current work is ongoing to further reduce surface damage during RIE to maximize the open circuit voltage and to optimize the deposition of a-Si:H on our bSi in order to reduce the loss in current density.

Tuning the thermoelectric properties by manipulating copper in Cu₂SnSe₃ system

\( \text{Cu}_2\text{x+x} \text{SnSe}_3 \) (0≤x≤0.08) compounds were synthesized by conventional solid-state reaction followed by spark plasma sintering (SPS) technique. Transport properties of the samples were measured as a function of temperature in the temperature range 323–773K. As compared to \( \text{Cu}_2\text{SnSe}_3 \) sample, the electrical resistivity (\( \rho \)) is increased for the sample with \( x=0.04 \), thereafter a decrease is seen with further increase in copper content. Analysis of electrical resistivity indicates that small polaron hopping model is operative in the entire temperature range for all samples. The positive Seebeck coefficient (S) for the samples in the entire temperature range indicates that the majority charge carriers are holes. The highest figure of merit, ZT (≈ 0.32) was achieved at 773K for the sample \( \text{Cu}_2\text{.06SnSe}_3 \) which is about 3 times that of \( \text{Cu}_2\text{SnSe}_3 \) sample. Maximum thermoelectric compatibility factor (\( \sim 1.28 V^{-1} \)) was observed at 673K for the sample \( \text{Cu}_2\text{.08SnSe}_3 \).
Tuning the Two-Dimensional Electron Gas at Oxide Interfaces with Ti-O Configurations: Evidence from X-ray Photoelectron Spectroscopy

Chemical redox reaction can lead to a two-dimensional electron gas (2DEG) at the interface between a TiO2-terminated SrTiO3 (STO) substrate and an amorphous LaAlO3 (a-LAO) capping layer. When replacing the STO substrate with rutile and anatase TiO2 substrates, considerable differences in interfacial conduction are observed. Based on X-ray photoelectron spectroscopy (XPS) and transport measurements, we conclude that the interfacial conduction comes from redox reactions, and that the differences among the materials systems result mainly from variations in the activation energies for the diffusion of oxygen vacancies at substrate surfaces.
Two level undercut-profile substrate-based filamentary coated conductors produced using metal organic chemical vapor deposition

The two level undercut-profile substrate (2LUPS) has been introduced as a concept for subdividing rare-earth-Ba$_2$Cu$_3$O$_{7}$ (REBCO) coated conductors (CC) into narrow filaments which reduces the AC losses and improves field stability for DC magnets. The 2LUPS consists of two levels of plateaus connected by a wall with an undercut-profile, which enables a physical separation of the superconducting layer between the plateaus without reducing the effective width of the superconducting layer. In this study we report for the first time the results of fabrication and characterization of a filamentary CC produced in an industrial setup by SuperPower Inc. using ion beam assisted deposition and metal organic chemical vapor deposition (IBAD-MOCVD) on a 2LUPS substrate realized at the Technical University of Denmark (DTU), whereas previous studies discussed the fabrication using alternating beam assisted deposition and pulsed laser deposition (ABAD-PLD). We also present Hall probe scanning measurements performed using a standard TAPESTAR® XL machine that is routinely employed for industrial critical current characterization of long length CCs. It clear that additional analysis of the measured field profiles are required when characterizing filamentary 2LUPS CC using a standard TAPESTAR® setting. Using FEM we calculated the expected magnetization response and we find a good agreement.

General information
State: Published
Number of pages: 5
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information
Journal: IEEE Transactions on Applied Superconductivity
Volume: 28
Issue number: 4
Article number: 6601705
ISSN (Print): 1051-8223
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 1.45 SJR 0.408 SNIP 0.962
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.42 SJR 0.398 SNIP 1.145
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.403 SNIP 1.06 CiteScore 1.27
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.478 SNIP 1.13 CiteScore 0.83
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.443 SNIP 1.156 CiteScore 1.32
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.555 SNIP 1.274 CiteScore 1.11
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Utilizing thermal building mass for storage in district heating systems: Combined building level simulations and system level optimization

Higher shares of intermittent renewable energy in energy systems have raised the issue of the need for different energy storage solutions. The utilization of existing thermal building mass for storage is a cost-efficient solution. In order to investigate its potential, a detailed building simulation model was coupled with a linear optimization model of the energy system. Different building archetypes were modelled in detail, and their potential preheating and subsequent heat supply cut-off periods were assessed. Energy system optimization focused on the impact of thermal mass for storage on the energy supply of district heating. Results showed that longer preheating time increased the possible duration of cut-off events. System optimization showed that the thermal mass for storage was used as intra-day storage. Flexible load accounted for 5.5%–7.7% of the total district heating demand. Furthermore, thermal mass for storage enabled more solar thermal heating energy to be effectively utilized in the system. One of the sensitivity analyses showed that the large-scale pit thermal energy storage and thermal mass for storage are complimentary. The cut-off duration potential, which did not compromise thermal comfort, was longer in the newer, better insulated buildings, reaching 6h among different building archetypes.

General information

State: Published
Organisations: Department of Energy Conversion and Storage, Department of Civil Engineering, Section for Indoor Climate and Building Physics, Department of Management Engineering, Systems Analysis, Centre for IT-Intelligent Energy Systems in Cities
Authors: Dominkovic, D. F. (Intern), Gianniou, P. (Intern), Münster, M. (Intern), Heller, A. (Intern), Rode, C. (Intern)
Pages: 949-966
Publication date: 2018
Main Research Area: Technical/natural sciences
Vapor pressure and specific electrical conductivity in the solid and molten H$_2$O-CsH$_2$PO$_4$-CsPO$_3$ system—a novel electrolyte for water electrolysis at ~225–400 °C

Cesium dihydrogen phosphate, CsH$_2$PO$_4$ (CDP) was studied for water electrolysis at ~225–400 °C. In the presence of sufficient humidity, CDP is structurally disordered and super-protonic conducting with conductivities reaching 0.2–0.25 S cm$^{-1}$, when determined in suitable H-shaped sealed conductivity cells. Freshly prepared 99.7 ± 0.3% gravimetric pure CDP with correct X-ray diffraction and DSC diagram melted at ~345 °C. The vapor pressures, above CDP alone and mixed with 20–50 mol% CsPO$_3$ or 13 mol% H$_2$O, were determined in sealed ampoules up to 355 °C by means of Raman spectroscopy based on internal reference gases. Pressures up to ~49 bar were estimated, much higher than previously expected. Conductivities were given as polynomials and plotted in solid and liquid states. Water splitting electrolysis 2H$_2$O $\rightarrow$ 2H$_2$ + O$_2$ was demonstrated by Raman at ~355 °C under a water pressure of ~23 bar in a quartz cell with platinum electrodes, showing molten CDP to have significant potential for water electrolysis.
Which Storage Types are Needed in Future Smart Energy Cities?

In future smart energy cities, storage technologies will play an important role in integration of intermittent energy sources. As many different storage technologies exist, such as chemical storage for electricity, heat/cold storage, hydrogen and methane storage and battery storage in electric vehicles, research was carried out in order to find the optimal combination of different storages in energy supply of future cities. A holistic energy system of a densely populated city in a hot climate was modelled including integrated power, cooling, gas and mobility sectors. A linear optimization model was used to detect the optimal capacities of different storage technologies, based on the minimization of the total socio-economic costs. The presented results showed the different optimal capacities of storages in different scenarios, as well as the influence of individual cooling versus district cooling on optimal storage capacities. In scenarios dominated by individual cooling, grid battery storage had significant installed capacities. However, scenarios dominated by district cooling showed that cheaper solutions can be obtained by using other storage solutions, such as cold energy storage.

Zirconia UV-curable colloids for additive manufacturing via hybrid inkjet printing-stereolithography

Currently, additive manufacturing of ceramics by stereolithography (SLA) is limited to single materials and by a poor thickness resolution that strongly depends on the ceramic particles-UV light interaction. Combining selective laser curing with inkjet printing represents a novel strategy to overcome these constrains. Nonetheless, this approach requires UV-curable inks that allow hardening of the printed material and sintering to high density. In this work, we report how to design an ink for inkjet printing of yttria stabilized zirconia (YSZ) which can be impressed by addition of UV-curable monomers. We especially show how the formulation of the inks and particularly the UV-monomer concentration impacts the printability and the UV-curing. This leads to prints that are resistant to solvent washing first and densely 96% dense YSZ layers after sintering.
Inkjet printing, UV-curable, Zirconia, Sintering
METHOD AND APPARATUS FOR CHARACTERIZATION OF A SOLAR CELL

The present disclosure relates to a method for characterization of a solar cell, comprising the steps of: providing an optical probe light; modulating the optical probe light with a modulation frequency of between 100 kHz and 50 MHz, thereby obtaining a modulated probe light; scanning the modulated probe light such that said modulated probe light is incident on at least a part of the surface of the solar cell, and such that the part of the solar cell exposed to the modulated probe light converts the modulated probe light to an electrical signal; detecting and analyzing said electrical signal; and estimating variations in the solar cell, thereby electrically characterizing the solar cell. The disclosure further relates to a solar cell characterization apparatus for characterization of a solar cell, comprising: a light source for generating an optical probe light; a modulation unit, configured to produce modulated probe light by modulating the optical probe light with a modulation frequency of between 100 kHz and 0 MHz; a light scanning unit for scanning the modulated probe light such that said modulated probe light is incident on at least a part of the surface of the solar cell; and a signal analyzer, configured to detect and analyze electrical signals produced by the solar cell as a response to exposure of the modulated probe light.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Organic Energy Materials
Authors: Krebs, F. C. (Intern)
Publication date: 16 Mar 2017

Publication information
IPC: H02S 50/15 A I
Patent number: WO2017042248
Date: 18/03/2017
Priority date: 08/09/2015
Priority number: EP20150184224
Original language: English
Electronic versions:
WO2017042248A1.pdf
Main Research Area: Technical/natural sciences
Source: espacenet
Source-ID: WO2017042248
Publication: Research › Patent – Annual report year: 2017

Durable fuel electrode

The present invention relates to a composite for an electrode, a composite precursor, a method of manufacturing a composite, and the composite obtained by said method. The invention further relates to an electrode comprising the composite, as well as a solid state electrochemical cell comprising the composite. The invention also relates to the use of the composite as a fuel electrode, solid oxide fuel cell, and/or solid oxide electrolyser. The invention discloses a composite for an electrode, comprising a three-dimensional network of dispersed metal particles, stabilised zirconia particles and pores, wherein the size of the pores is smaller than the size of the metal particles, wherein the size of the metal particles is essentially equal to or smaller than the size of the stabilised zirconia particles, wherein the porosity is below 33, 30, or 29 vol%, more preferably below 26 or 24 vol%, and most preferably below 23, 22, 21, 18, 15, or 13 vol%, and/or wherein the pores are essentially exclusively generated from the volume created by reducing a corresponding metal oxide to the metal particles.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Applied Electrochemistry, Mixed Conductors
Authors: Brodersen, K. (Intern), Hauch, A. (Intern), Chen, M. (Intern), Hjelm, J. (Intern)
Publication date: 23 Feb 2017

Publication information
IPC: H01M 8/124 A I
Patent number: WO2017029350
3D printed barium titanate/poly-(vinylidene fluoride) nano-hybrid with anisotropic dielectric properties

Electrospun BaTiO$_3$ nanofibers (BTNFs) are synthesized and blended in a poly(vinylidene fluoride) (PVDF) matrix to obtain a flexible nano-hybrid composite with high dielectric constant (flexible high-k). The blending is performed with different BTNF contents (0.6, 4.5, 20 vol%). The rheological properties of the starting materials are optimized to shape the hybrid by the precision-extrusion-based fuse deposition modeling technique. The 3D-printed BTNFs allow complex shapes with different degrees of fiber alignment as the result of printing shear stress and the chemical composition of the starting material. The dielectric properties of the nano-hybrid are controlled by anisotropy with an enhancement in the nanofiber cross direction (⊥), where the dielectric constant $k_{\perp}$ at 1 kHz is increased to ca. 200 from 13 of the PVDF matrix.

**General information**

State: Published
Organisations: Department of Energy Conversion and Storage, Imaging and Structural Analysis, Ceramic Engineering & Science, Technical University of Denmark, Silpakorn University, Universidade Federal do ABC
Authors: Phatharapeetranun, N. (Ekstern), Ksapabutr, B. (Ekstern), Marani, D. (Ekstern), Bowen, J. R. (Intern), Esposito, V. (Intern)
Pages: 12430-12440
Publication date: 2017
Main Research Area: Technical/natural sciences

**Publication information**

Journal: Journal of Materials Chemistry C
Volume: 5
Issue number: 47
ISSN (Print): 2050-7526
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 1.3 SJR 1.917 CiteScore 5.67
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 5.14 SJR 1.825 SNIP 1.266
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.713 SNIP 1.508 CiteScore 5.32
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.517 SNIP 1.351 CiteScore 4.64
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
ISI indexed (2013): ISI indexed no
Original language: English
Electronic versions:
c7tc03697c.pdf
DOIs:
10.1039/c7tc03697c
Source: PublicationPreSubmission
Source-ID: 139763349
Publication: Research - peer-review › Journal article – Annual report year: 2017
Acid-base chemistry and proton conductivity of CsHSO$_4$, CsH$_2$PO$_4$ and their mixtures with N-heterocycles

Caesium hydrogen sulfate (CsHSO$_4$) and caesium dihydrogen phosphate (CsH$_2$PO$_4$) are solid acids that undergo superprotonic phase-transitions at about 140 and 230 °C, respectively. As a result, the proton conductivity is increased by several orders of magnitude. However, the practical operational temperature range is narrow due to decomposition of the high-conductivity phases. For CsHSO$_4$, it is known that this window can be extended to lower temperatures by addition of carefully selected N-heterocycles. The present work investigates if the same approach can be used to extend the practical operating temperature range of CsH$_2$PO$_4$ as well. Binary mixtures of CsH$_2$PO$_4$ with 1,2,4-triazole, benzimidazole or imidazole were prepared by means of mechanochemical synthesis. Mixtures based on CsHSO$_4$ were prepared as a basis for a comparative discussion. It was found that CsHSO$_4$ formed organic-inorganic salts, while CsH$_2$PO$_4$ formed heterogeneous mixtures with the N-heterocycles due to its weaker acidity. At a N-heterocycle content of 30 mol%, enhanced proton conductivity was observed for both solid acids at temperatures below their superprotonic phase transitions.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors
Authors: Aili, D. (Intern), Gao, Y. (Intern), Han, J. (Intern), Li, Q. (Intern)
Pages: 13-19
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Solid State Ionics
Volume: 306
ISSN (Print): 0167-2738
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 2.64 SJR 0.856 SNIP 0.952
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.41 SJR 0.75 SNIP 0.909
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.802 SNIP 1.016 CiteScore 2.5
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.837 SNIP 1.282 CiteScore 2.62
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.903 SNIP 1.269 CiteScore 2.35
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.051 SNIP 1.253 CiteScore 2.31
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.376 SNIP 1.615 CiteScore 2.96
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.46 SNIP 1.498
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.508 SNIP 1.483
A Contribution to the Understanding of the Combined Effect of Nitrogen and Boron in Grey Cast Iron

Inoculation is an essential part of controlling material properties in grey cast iron. Inoculation practice has for decades been based on the addition to the melt of small amounts of elements with a strong affinity to O (and S) just before casting takes place. This method is proven—both in theory and in practice—to be effective in most cases. But it has the disadvantage that the nucleation effect fades away over time. In particular, in heavy castings (slow cooling) this effect may cause non-uniform and unacceptable material properties in some parts of the casting. Nitrogen is also known to influence grey iron microstructure. Both graphite flake formation and matrix formation are influenced. However, the obtained effects differ considerably between different reported investigations. This investigation deals with the combined effect of nitrogen and boron and how it is possible to utilize this effect to enhance material properties in heavy grey iron castings. It is shown that the controlled additions of nitrogen and boron can be used to control the microstructure of thick section grey iron castings. A plausible theory for the formation of boron nitride nuclei effective for graphite growth is presented.

General information

State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Department of Mechanical Engineering, Manufacturing Engineering, Dansk Udviklings Formidling ApS
Authors: Strande, K. (Ekstern), Tiedje, N. S. (Intern), Chen, M. (Intern)
Number of pages: 10
Pages: 61-70
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information

Journal: International Journal of Metalcasting
Volume: 11
Issue number: 1
ISSN (Print): 1939-5981
Ratings:

Web of Science (2018): Indexed yes
Scopus rating (2017): CiteScore 0.66 SJR 0.329 SNIP 0.729
Web of Science (2017): Indexed yes
Scopus rating (2016): CiteScore 0.47 SJR 0.304 SNIP 0.688
Addressing uncertainty in atomistic machine learning

Machine-learning regression has been demonstrated to precisely emulate the potential energy and forces that are output from more expensive electronic-structure calculations. However, to predict new regions of the potential energy surface, an assessment must be made of the credibility of the predictions. In this perspective, we address the types of errors that might arise in atomistic machine learning, the unique aspects of atomistic simulations that make machine-learning challenging, and highlight how uncertainty analysis can be used to assess the validity of machine-learning predictions. We suggest this will allow researchers to more fully use machine learning for the routine acceleration of large, high-accuracy, or extended-time simulations. In our demonstrations, we use a bootstrap ensemble of neural network-based calculators, and show that the width of the ensemble can provide an estimate of the uncertainty when the width is comparable to that in the training data. Intriguingly, we also show that the uncertainty can be localized to specific atoms in the simulation, which may offer hints for the generation of training data to strategically improve the machine-learned representation.
A Decade of Solid Oxide Electrolysis Improvements at DTU Energy

Solid oxide electrolysis cells (SOECs) can efficiently convert electrical energy (e.g. surplus wind power) to energy stored in fuels such as hydrogen or other synthetic fuels. Performance and durability of the SOEC has increased orders of magnitudes within the last decade. This paper presents a short review of the R&D work on SOEC single cells conducted at DTU Energy from 2005 to 2015. The SOEC improvements have involved increasing the of the oxygen electrode performance, elimination of impurities in the feed streams, optimization of processing routes, and fuel electrode structure optimization. All together, these improvements have led to a decrease in long-term degradation rate from ~40 %/kh to ~0.4
%/kh for steam electrolysis at -1 A/cm², while the initial area specific resistance has been decreased from 0.44 Ωcm² to 0.15 Ωcm² at -0.5 A/cm² and 750 °C.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry, Ceramic Engineering & Science, Mixed Conductors, Imaging and Structural Analysis
Number of pages: 12
Pages: 3-14
Publication date: 2017
Conference: PRIME 2016/230th ECS Meeting, Honolulu, United States, 02/10/2016 - 02/10/2016
Main Research Area: Technical/natural sciences

Publication information
Journal: ECS Transactions
Volume: 75
Issue number: 42
ISSN (Print): 1938-6737
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 0.44 SJR 0.225 SNIP 0.252
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 0.4 SJR 0.228 SNIP 0.253
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.211 SNIP 0.244 CiteScore 0.36
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.212 SNIP 0.234 CiteScore 0.36
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.192 SNIP 0.231 CiteScore 0.27
ISI indexed (2013): ISI indexed no
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.241 SNIP 0.26 CiteScore 0.29
ISI indexed (2012): ISI indexed no
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.261 SNIP 0.28 CiteScore 0.36
ISI indexed (2011): ISI indexed no
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.249 SNIP 0.251
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.242 SNIP 0.27
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.254 SNIP 0.255
Scopus rating (2007): SJR 0.213 SNIP 0.206
Scopus rating (2006): SJR 0.134 SNIP 0.073
Original language: English
Electronic versions:
Hauch_A_Decade_of_SOEC_Improvements_at_DTU_Energy_20161026_after_review.pdf
DOIs:
10.1149/07542.0003ecst

Bibliographical note
doi: 10.1149/07542.0003ecst
Source: PublicationPreSubmission
Source-ID: 128494116
Publication: Research - peer-review > Conference article – Annual report year: 2017
A density functional theory study of the carbon-coating effects on lithium iron borate battery electrodes

Lithium iron borate (LiFeBO3) is a promising cathode material due to its high theoretical specific capacity, inexpensive components and a small volume change during operation. Yet, challenges relating to severe air- and moisture-induced degradation necessitate the application of a protective coating on the electrode which also improves the electronic conductivity. However, not much is known about the preferential geometries of the coating as well as how these coating–electrode interfaces influence the lithium diffusion between the coating and the electrode. Here, we therefore present a density functional theory (DFT) study of the anchoring configurations of carbon coating on the LiFeBO3 electrode and its implications on the interfacial lithium diffusion. Due to large barriers associated with Li-ion diffusion through a parallel-oriented pristine graphene coating on the FeBO3 and LiFeBO3 electrode surfaces, large structural defects in the graphene coating are required for fast Li-ion diffusion. However, such defects are expected to exist only in small concentrations due to their high formation energies. Alternative coating geometries were therefore investigated, and the configuration in which the graphene coating layers were anchored normal to the electrode surface at B and O atoms were found to be most stable. Nudged elastic band (NEB) calculations of the lithium diffusion barriers across the interface between the optimally oriented coating layers and the electrode show no kinetic limitations for lithium extraction and insertion. Additionally, this graphite-coating configuration showed partial blocking of electrode-degrading species.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials
Authors: Loftager, S. (Intern), García Lastra, J. M. (Intern), Vegge, T. (Intern)
Pages: 2087-2094
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Physical Chemistry Chemical Physics
Volume: 19
ISSN (Print): 1463-9076
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 4.04 SJR 1.686 SNIP 1.089
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.06 SJR 1.685 SNIP 1.113
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.725 SNIP 1.205 CiteScore 4.45
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.771 SNIP 1.239 CiteScore 4.29
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.72 SNIP 1.207 CiteScore 4.05
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.921 SNIP 1.177 CiteScore 3.67
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.707 SNIP 1.19 CiteScore 3.6
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.817 SNIP 1.199
A Durability Study of High-temperature PEMFC. Effects of Operating Parameters and Thermal Curing

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors, Department of Mechanical Engineering, Materials and Surface Engineering, Danish Power Systems ApS
Authors: Jensen, J. O. (Intern), Søndergaard, T. (Intern), Aili, D. (Intern), Steenberg, T. (Ekstern), Hjuler, H. A. (Ekstern), Becker, H. (Intern), Zhong, L. (Intern), Li, Q. (Intern)
Number of pages: 1
Publication date: 2017
Event: Abstract from 5th International CARISMA Conference (2017), Newcastle, United Kingdom.
Main Research Area: Technical/natural sciences
Electronic versions:
Carisma_2017_Abstract_Jens_Oluf_Jensen_1.pdf
Source: PublicationPreSubmission
Source-ID: 141975367
Publication: Research › Conference abstract for conference – Annual report year: 2017

Advanced fabrication of porous ceramic multilayers for membrane applications

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Proton conductors, Department of Biotechnology and Biomedicine, Department of Chemical and Biochemical Engineering
Advanced manufacturing of porous ceramic structures for use in energy applications (invited)

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Proton conductors, Mixed Conductors
Authors: Kaiser, A. (Intern), Bjørnetun Haugen, A. (Intern), Zhang, W. (Intern), Ovtar, S. (Intern), Kiebach, W. (Intern), Hendriksen, P. V. (Intern)
Pages: 11
Publication date: 2017

A facile approach to fabricate hierarchically structured poly(3-hexylthiophene-2,5-diyl) films

Microstructured surfaces have great potentials to improve the performances and efficiency of optoelectronic devices. In this work, a simple robust approach based on surface instabilities was presented to fabricate poly(3-hexylthiophene-2,5-diyl) (P3HT) films with ridge-like/wrinkled composite microstructures. Namely, the hierarchically patterned films were prepared by spin coating the P3HT/tetrahydrofuran (THF) solution on a polydimethylsiloxane (PDMS) substrate to form stable ridge-like structures, followed by solvent vapor swelling to create surface wrinkles with the orientation guided by the ridge-like structures. During spin coating of the P3HT/THF solution, the ridge-like structures were generated by the in-situ template of the THF swelling-induced creasing structures on the PDMS substrate. To our knowledge, it is the first report that the creasing structures are used as a recoverable template for patterning films. The crease-templated ridge-like structures were well modulated by the THF swelling time, the modulus of the PDMS substrate, the P3HT/THF solution concentration and the selective/blanket exposure of the PDMS substrate to O2 plasma. UV–vis and fluorescence spectrometry measurements indicated that the light absorption and fluorescent emission were improved on the hierarchically patterned P3HT films, which can be utilized to enhance the efficiencies of organic solar cells. Furthermore, this simple versatile method based on the solvent swelling-induced crease as the in-situ recoverable template has been extended to pattern other spin-coated films with different compositions.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Imaging and Structural Analysis, Tianjin University, Chinese Academy of Sciences
Pages: 928-939
Publication date: 2017
Main Research Area: Technical/natural sciences
Volume: 55
Issue number: 12
ISSN (Print): 0887-6266
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 0.88 SJR 0.837 CiteScore 2.52
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.12 SJR 1.067 SNIP 0.97
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.235 SNIP 1.117 CiteScore 3.4
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.503 SNIP 1.412 CiteScore 3.91
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.185 SNIP 1.3 CiteScore 3
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.067 SNIP 1.168 CiteScore 2.29
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.788 SNIP 0.906 CiteScore 1.74
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.903 SNIP 0.959
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.156 SNIP 1.005
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.143 SNIP 1.112
Scopus rating (2007): SJR 1.24 SNIP 1.132
Scopus rating (2006): SJR 1.267 SNIP 1.245
Scopus rating (2005): SJR 1.202 SNIP 1.054
Scopus rating (2004): SJR 1.287 SNIP 1.243
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.268 SNIP 1.248
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 1.256 SNIP 1.165
Scopus rating (2001): SJR 1.436 SNIP 1.369
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 1.423 SNIP 1.467
Scopus rating (1999): SJR 1.481 SNIP 1.401
Original language: English
Light harvesting efficiency;, Oxygen plasma treatment, Poly(3-hexylthiophene-2,5-diyl) films, Surface instability, Surface microstructures
DOIs:
10.1002/polb.24339
Source: FindIt
Source-ID: 2358319569
Publication: Research - peer-review › Journal article – Annual report year: 2017
A Fully Developed Flow Thermo-fluid Model for Topology Optimization of 3D-Printed Air-Cooled Heat Exchangers

In this work, density-based topology optimization is applied to the design of the air-side surface of dry-cooled power plant condensers. A topology optimization model assuming a steady-state, thermally and fluid dynamically fully developed internal flow is developed and used for this application. The conductance of the heat exchanger is maximized for a prescribed pressure drop and prescribed air-side temperature change across the heat exchanger. Polymer with infilled thermally conducting metal filaments is considered as the heat exchanger material which allows cost effective additive manufacturing techniques to be used to fabricate the obtained designs. Parametric studies are presented that analyze the effect of the material thermal conductivity and the heat exchanger unit cell height on the system's performance. The designs obtained from topology optimization are benchmarked against a simple optimized slot channel model in order to demonstrate the superior performance of the topology optimized designs. Thus, this work demonstrates the usefulness of topology optimization to fully exploit the design freedom afforded by additive manufacturing technologies.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, University of Wisconsin-Madison
Authors: Haertel, J. H. K. (Intern), Nellis, G. F. (Ekstern)
Pages: 10-24
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Applied Thermal Engineering
Volume: 119
ISSN (Print): 1359-4311
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 4.14 SJR 1.505 SNIP 1.837
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.78 SJR 1.438 SNIP 1.851
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.683 SNIP 1.884 CiteScore 3.32
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.539 SNIP 2.187 CiteScore 3.16
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.466 SNIP 2.469 CiteScore 3.31
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.492 SNIP 2.422 CiteScore 2.7
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.338 SNIP 2.186 CiteScore 2.83
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.385 SNIP 2.012
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.393 SNIP 2.105
Web of Science (2009): Indexed yes
Alkaline membrane water electrolysis with non-noble catalysts

As renewable energy sources reach higher grid penetration, large scale energy storage solutions are becoming increasingly important. Hydrogen produced with renewable energy by water electrolysis is currently the only option to solve this challenge on a global scale, and green hydrogen is essential for the decarbonization of the transportation and industrial sector required to limit climate change.

Electrolysis done with an alkaline electrolyte is a cheap, proven, and commercially available technology, but the systems suffer from inefficiency and limited operating flexibility. The work herein seek to address these issues by introducing alkaline polymeric membranes and efficient electrodes based on novel materials.

Polymer electrolyte membranes with sufficient OH⁻ conductivity enable a drastic reduction of the electrode spacing, which lead to improved ohmic properties enabling operation at higher current density. This, combined with better gas separation properties and a higher operating flexibility, have the prospects of significantly reducing the capex and opex of electrolysis systems, and the cost of green hydrogen. Towards this goal, membranes based on poly(2,2'-(m-phenylene)-5,5'-bibenzimidazole) (m-PBI) as well as poly(2,2'-(m-mesitylene)-5,5'-bibenzimidazole) (mes-PBI) were investigated as electrolyte for alkaline electrolysis cells.

PBI membranes were equilibrated with aqueous KOH and applied as separator, and polarization data from cells at 20-25 wt% KOH using these membranes showed improved ohmic behaviour over cells with conventional porous separators. This was strikingly clear when combined with active electrodes with Raney-nickel-based coatings. With thin 40 μm m-PBI membranes, Raney-nickel-molybdenum cathodes and nickel anodes, cells operated at 80 °C with 24 wt% KOH (aq) achieved 1000 mA cm⁻² at 1.7 V and 2800 mA cm⁻² at 2.0 V. Electrochemical impedance spectroscopy data showed a 6-fold reduction in ohmic cell resistance compared to conventional materials. Albeit good performance, ex-situ characterization and durability tests showed that polymer backbone and membrane stability remained a problem under conventional operating conditions.

To accompany novel membranes in alkaline electrolysis, electrodes can be employed in a zero-gap configuration. This enable different electrode concepts than used in commercial systems. Inspired by recent literature, nickel-iron based anodes, and nickel-tin as well as nickel-molybdenum cathodes were investigated in half cell tests. The materials were applied as coatings on nickel foam and showed improvements in the order of 150-300 mV over reference nickel materials at room temperature, depending on the specific electrode and electrolyte concentration used.

In a secondary approach, electrodes were prepared using powder and polymeric binders. Using nickel powder with m-PBI binder in a nickel foam as cathode, a reduction in cell overpotential of more than 200 mV was achieved compared against a pristine nickel foam cathode.
A multi-objective energy planning including system exergy efficiency and socio-economic costs

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Department of Mechanical Engineering, Thermal Energy
Authors: Dominkovic, D. F. (Intern), Pedersen, A. S. (Intern), Elmegaard, B. (Intern)
Number of pages: 1
Publication date: 2017

Host publication information
Title of host publication: Proceedings of ECOS 2017 - 30th International Conference on Efficiency, Cost, Optimisation, Simulation and Environmental Impact of Energy Systems
Main Research Area: Technical/natural sciences
Conference: 30th International Conference on Efficiency, Cost, Optimization, Simulation and Environmental Impact of Energy Systems (ECOS 2017), San Diego, United States, 02/07/2017 - 02/07/2017
Exergy, Energy planning, Multi-objective optimization, Socio-economic costs, Zero carbon, Pareto frontier
Electronic versions:
A_multi_objective_energy_planning_including_system_exergy_efficiency_and_socio_economic_costs_ABSTRACT.pdf
Source: PublicationPreSubmission
Source-ID: 139631442
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2017

Analysis of electrical and thermal stress effects on PCBM:P3HT solar cells by photocurrent and impedance spectroscopy modeling

We investigated the effects of electrical stress and thermal storage by means of photocurrent, Impedance Spectroscopy and Open Circuit Voltage Decay models. The electrical stress damages only the active layer, by reducing the generation rate, the polaron separation probability and the carrier lifetime. The thermal stress also degrades the anode interface. This reflects on the appearance of an inflection in the I-V photocurrent shape close to the operative region.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Organic Energy Materials, University of Padova
Authors: Torto, L. (Ekstern), Rizzo, A. (Ekstern), Cester, A. (Ekstern), Wrachien, N. (Ekstern), Passarini, L. (Ekstern), Krebs, F. C. (Intern), Corazza, M. (Intern), Gevorgyan, S. A. (Intern)
Number of pages: 10
Publication date: 2017

Host publication information
Title of host publication: Proceedings of the IEEE International Reliability Physics Symposium (IRPS 2017)
Publisher: IEEE
Article number: 2F-4
ISBN (Print): 978-1-5090-6640-7
Main Research Area: Technical/natural sciences
Conference: 2017 IEEE International Reliability Physics Symposium , Monterey, United States, 02/04/2017 - 02/04/2017
Organic solar cell reliability, Photocurrent models, Carrier lifetime
DOIs:
10.1109/IRPS.2017.7936274
Source: FindIt
Source-ID: 2371003466
Analysis of Gas Leakage and Current Loss of Solid Oxide Fuel Cells by Screen Printing
Two types of anode supported solid oxide fuel cell (SOFC) NiO-YSZ/YSZ/GDC/LSCF with the same structure and different manufacturing process were tested. Gas leakage was suspected for cells manufactured with screen printing technique. Effective leak current densities for both types of cells were calculated. Their performances of electrochemical impedance spectroscopy (EIS) were compared and distribution function of relaxation times (DRT) technique was also used to find the clue of gas leakage. Finally, thinning and penetrating holes were observed in electrolyte layer, which confirmed the occurrence of gas leakage.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Tsinghua University
Authors: Jia, C. (Ekstern), Han, M. (Ekstern), Chen, M. (Intern)
Pages: 1533-1540
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: E C S Transactions
Volume: 78
Issue number: 1
ISSN (Print): 1938-5862
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 0.44 SJR 0.225 SNIP 0.252
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 0.4 SJR 0.228 SNIP 0.253
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.211 SNIP 0.244 CiteScore 0.36
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.212 SNIP 0.234 CiteScore 0.36
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.192 SNIP 0.231 CiteScore 0.27
ISI indexed (2013): ISI indexed no
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.241 SNIP 0.26 CiteScore 0.29
ISI indexed (2012): ISI indexed no
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.261 SNIP 0.28 CiteScore 0.36
ISI indexed (2011): ISI indexed no
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.249 SNIP 0.251
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.242 SNIP 0.27
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.254 SNIP 0.255
Scopus rating (2007): SJR 0.213 SNIP 0.206
Scopus rating (2006): SJR 0.134 SNIP 0.073
Original language: English
Electronic versions:
DOIs:
10.1149/07801.1533ecst
**Analysis of Gas Leakage and Current Loss of Solid Oxide Fuel Cells by Screen Printing**

One of the biggest advantages of SOFC (solid oxide fuel cell) is the probable use of methane as fuel. However, when the actual SOFC stack is operating with CH$_4$ as fuel, due to the catalytic action of metal nickel, carbon will deposit on SOFC anode and nickel foam, which directly shorten the SOFC operating life and lead to performance degradation. The planar anode-supported Ni-YSZ|YSZ|LSCF SOFC was chosen as the research object, with the cell size of 12cm×12cm and the effective area of 100cm$^2$, and the holder is made of 99% purity of Al$_2$O$_3$ ceramic material, in order to eliminate the influence of Cr in stainless steel. The one-cell stack operated at 750°C, and the maximum power density was 0.35W/cm$^2$ when the fuel is 0.5slm/min pure hydrogen. The stability experiment was conducted first under pure H$_2$ for 100h, then fuel was switched into pure methane, and another 100h of voltage stability was tested. In this work, the temperature distribution of the stack was monitored, whose relationship with the weight gain and the micro-structure of the nickel foam was established, and a possible explanation of the carbon deposition distribution and process on the nickel foam was put forward.

**General information**
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Tsinghua University
Authors: Jia, C. (Ekstern), Han, M. (Ekstern), Chen, M. (Intern)
Pages: 1
Publication date: 2017
Conference: 15th International Symposium on Solid Oxide Fuel Cells (SOFC-XV), Hollywood, United States, 23/07/2017 - 23/07/2017
Main Research Area: Technical/natural sciences

**Publication information**
Journal: Electrochemical Society. Meeting Abstracts (Online)
Volume: MA2017-03
Article number: 87
ISSN (Print): 2151-2043
Original language: English
Links:
http://ma.ecsdl.org/content/MA2017-03/1/87.abstract

**Bibliographical note**
Poster Session I (Cathodes and Anodes)
Publication: Research - peer-review › Conference abstract in journal – Annual report year: 2017

**An effective low Pd-loading catalyst for hydrogen generation from formic acid**
As an interesting hydrogen carrier, formic acid is bio-renewable, non-toxic and available in the liquid state at room temperature. The development of active and low-cost catalyst is of significance for hydrogen generation from formic acid. In this study, both a relatively cheap metal (Ag) and a functional support (nitrogen modified reduced graphene oxide, N-rGO) were applied to prepare Pd catalyst. It was found that the Ag atoms facilitated the formation of Pd-rich surface in the preparation strategy, in which the reductive N-rGO and a two-step feeding process of metal precursors played important roles. In addition, Ag additive was found to benefit catalyst stability. Most interestingly, the obtained low Pd-loading Pd$_{1}$Ag$_{6}$/N-rGO catalyst showed a specific Pd loading turnover frequency of 171 mol Pd$^{-1}$ h$^{-1}$ and a specific metal cost turnover frequency of 64.2 $^{-1}$ h$^{-1}$, which were predominant among currently available Pd-based catalysts towards formic acid decomposition without any additive under room temperature.

**General information**
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors, China University of Geosciences, Wuhan
Authors: Huang, Y. (Ekstern), Xu, J. (Ekstern), Ma, X. (Ekstern), Huang, Y. (Ekstern), Li, Q. (Intern), Qiu, H. (Ekstern)
Pages: 18375-18382
Publication date: 2017
Main Research Area: Technical/natural sciences

**Publication information**
Volume: 42
Issue number: 29
ISSN (Print): 0360-3199
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
A new method to measure mechanics and dynamic assembly of branched actin networks

We measured mechanical properties and dynamic assembly of actin networks with a new method based on magnetic microscopic cylinders. Dense actin networks are grown from the cylinders' surfaces using the biochemical Arp2/3-
machinery at play in the lamellipodium extension and other force-generating processes in the cell. Under a homogenous magnetic field the magnetic cylinders self-assemble into chains in which forces are attractive and depend on the intensity of the magnetic field. We show that these forces, from piconewtons to nanonewtons, are large enough to slow down the assembly of dense actin networks and controlled enough to access to their non linear mechanical responses. Deformations are measured with nanometer-resolution, well below the optical resolution. Self-assembly of the magnetic particles into chains simplifies experiments and allows for parallel measurements. The combination of accuracy and good throughput of measurements results in a method with high potential for cell and cytoskeleton mechanics. Using this method, we observed in particular a strong non linear mechanical behavior of dense branched actin networks at low forces that has not been reported previously.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, ESPCI Paris, Universitat Pompeu Fabra
Authors: Bauër, P. (Ekstern), Tavacoli, J. (Intern), Pujol, T. (Ekstern), Planade, J. (Ekstern), Heuvingh, J. (Ekstern), Du Roure, O. (Ekstern)
Number of pages: 11
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Scientific Reports
Volume: 7
Article number: 15688
ISSN (Print): 2045-2322
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 4.36 SJR 1.533 SNIP 1.245
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.63 SJR 1.692 SNIP 1.354
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 2.034 SNIP 1.597 CiteScore 5.3
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.163 SNIP 1.554 CiteScore 4.75
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.998 SNIP 1.57 CiteScore 4.06
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.531 SNIP 0.962 CiteScore 2.44
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
ISI indexed (2011): ISI indexed no
Original language: English
Electronic versions:
s41598_017_15638_5orb.pdf
DOIs:
10.1038/s41598-017-15638-5
Source: PublicationPreSubmission
Source-ID: 139557206
Publication: Research - peer-review › Journal article – Annual report year: 2017
Anisotropic Proton and Oxygen Ion Conductivity in Epitaxial Ba$_2$In$_2$O$_5$ Thin Films

Solid oxide oxygen ion and proton conductors are a highly important class of materials for renewable energy conversion devices like solid oxide fuel cells. Ba$_2$In$_2$O$_5$ (BIO) exhibits both oxygen ion and proton conduction, in a dry and humid environment, respectively. In a dry environment, the brownmillerite crystal structure of BIO exhibits an ordered oxygen ion sublattice, which has been speculated to result in anisotropic oxygen ion conduction. The hydrated structure of BIO, however, resembles a perovskite and the protons in it were predicted to be ordered in layers. To complement the significant theoretical and experimental efforts recently reported on the potentially anisotropic conductive properties in BIO, we measure here both the proton and oxygen ion conductivity along different crystallographic directions. Using epitaxial thin films with different crystallographic orientations, the charge transport for both charge carriers is shown to be anisotropic. The anisotropy of the oxygen ion conduction can indeed be explained by the layered structure of the oxygen sublattice of BIO. The anisotropic proton conduction, however, further supports the suggested ordering of the protonic defects in the material. The differences in proton conduction along different crystallographic directions attributed to proton ordering in BIO are of a similar extent as those observed along different crystallographic directions in materials where proton ordering is not present but where protons find preferential conduction pathways through chainlike or layered structures.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Department of Physics, Atomic scale modelling and materials, Paul Scherrer Institut, Chalmers University of Technology, University of Göttingen, University of Verona
Authors: Fluri, A. (Ekstern), Gilardi, E. (Ekstern), Karlsson, M. (Ekstern), Roddatis, V. (Ekstern), Bettinelli, M. (Ekstern), Castelli, I. E. (Intern), Lippert, T. (Ekstern), Pergolesi, D. (Ekstern)
Pages: 21797–21805
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: The Journal of Physical Chemistry Part C
Volume: 121
Issue number: 40
ISSN (Print): 1932-7447
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 4.58 SJR 2.135 SNIP 1.147
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.48 SJR 1.964 SNIP 1.195
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.886 SNIP 1.26 CiteScore 4.68
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.032 SNIP 1.447 CiteScore 5.08
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 2.143 SNIP 1.445 CiteScore 5.14
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.529 SNIP 1.461 CiteScore 4.98
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.339 SNIP 1.465 CiteScore 4.92
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
A Novel SOFC/SOEC Sealing Glass with a Low SiO₂ Content and a High Thermal Expansion Coefficient

Solid oxide cells require seals that can function in harsh, elevated temperature environments. In addition, a low Si content can be advantageous, since Si impurities from the glass sealant can be transported to the active fuel electrode and poison the Ni-YSZ triple phase boundaries. To reduce the amount of Si emission, a low Si containing sealing glass (chemical composition: 50 mol% CaO, 20 mol% ZnO, 20 mol% B₂O₃ and 10 mol% SiO₂) was developed at DTU. In this work, the results from thermal characterization, the crystallization behavior of the glass and the long-term stability and adhesion behavior of the glass were studied under SOFC and SOEC relevant conditions. The glass-ceramic sealant performed well over 400 h, and no cell degradation or leakage related to the seal was found, indicating that the developed glass system is applicable for the use in SOFC/SOEC stacks.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors
Authors: Kiebach, W. (Intern), Agersted, K. (Ekstern), Zielke, P. (Intern), Ritucci, I. (Intern), Brock, M. B. (Intern), Hendriksen, P. V. (Intern)
Pages: 1739-1747
Publication date: 2017
Conference: 15th International Symposium on Solid Oxide Fuel Cells (SOFC-XV), Hollywood, United States, 23/07/2017 - 23/07/2017
Main Research Area: Technical/natural sciences

Publication information
Journal: ECS Transactions
Volume: 78
Issue number: 1
ISSN (Print): 1938-5862
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 0.44 SJR 0.225 SNIP 0.252
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 0.4 SJR 0.228 SNIP 0.253
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.211 SNIP 0.244 CiteScore 0.36
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.212 SNIP 0.234 CiteScore 0.36
A Novel SOFC/SOEC Sealing Glass with a Low SiO₂ Content and a High Thermal Expansion Coefficient

Solid oxide cells require seals that can function in harsh, elevated temperature environments. In the case of solid oxide electrolysis (SOEC), also a low Si content is desired, since Si impurities from the glass sealing can be transported to the active fuel electrode and poison the Ni-YSZ triple phase boundaries.

To reduce the amount of Si emission, a low Si containing sealing glass (chemical composition: 48 mol% CaO, 19 mol% ZnO, 21 mol% B₂O₃ and 12 mol% SiO₂) was developed at DTU. In this presentation, the results from thermal characterization, like thermal expansion coefficient, glass transition temperature, crystallization temperature, etc., of the glass will be presented. Additionally, the crystallization behavior of the glass was analyzed by in-situ X-ray diffraction, recording temperature resolved XRD spectra from 30 °C up to 900 °C.

Furthermore, the long-term stability and the adhesion behavior of the glass were studied under relevant SOFC and SOEC conditions. The stability of sealed Crofer/Glass/NiO-YSZ assemblies in reducing atmosphere and in air was investigated for over 500 h at temperatures between 750 °C and 850 °C. Additionally, a cell component test was performed to investigate the durability of the glass seal when exposed to dual atmosphere environments. The seals performed well over 400 h under fuel cell and electrolysis operation conditions, and no cell degradation or leakage related to the sealing was found, indicating that the developed glass system is applicable for the use in SOFC/SOEC stacks.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Office for Research and Relations
Authors: Kiebach, W. (Intern), Agersted, K. (Ekstern), Zielke, P. (Intern), Ritucci, I. (Intern), Brock, M. B. (Intern), Hendriksen, P. V. (Intern)
Pages: 1
Publication date: 2017
Conference: 15th International Symposium on Solid Oxide Fuel Cells (SOFC-XV), Hollywood, United States, 23/07/2017 - 23/07/2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Electrochemical Society. Meeting Abstracts (Online)
Volume: MA2017-03
Article number: 137
ISSN (Print): 2151-2043
Original language: English
Links:
http://ma.ecsdl.org.proxy.findit.dtu.dk/content/MA2017-03/1/137.abstract
Publication: Research - peer-review › Conference abstract in journal – Annual report year: 2017
A Physically-Based Equivalent Circuit Model for the Impedance of a LiFePO$_4$/Graphite 26650 Cylindrical Cell

In this work an Equivalent Circuit Model (ECM) is developed and used to model impedance spectra measured on a commercial 26650 LiFePO$_4$/Graphite cylindrical cell. The ECM is based on measurements and modeling of impedance spectra recorded separately on cathode (LiFePO$_4$) and anode (Graphite) samples, harvested from the commercial cell. Modeling of the single-electrode impedance spectra provided information about the electronic and ionic resistance in the porous composite electrodes, as well as the solid state diffusion. Focused Ion Beam (FIB)/Scanning Electron Microscopy (SEM) of anode and cathode samples was used to make 3-D maps of the electrode microstructures and to obtain microstructural data for the ECM. The complementary analysis was crucial for the resolution of the single electrode impedance parameters and the proposal and validation of a new equivalent circuit used to model the full commercial battery impedance.

General information

State: Published
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry, Imaging and Structural Analysis
Authors: Scipioni, R. (Intern), Jørgensen, P. S. (Intern), Graves, C. R. (Intern), Hjelm, J. (Intern), Jensen, S. H. (Intern)
Pages: A2017-A2030
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information

Journal: Journal of The Electrochemical Society
Volume: 164
Issue number: 9
ISSN (Print): 0013-4651
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 3.48 SJR 1.267 SNIP 1.009
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.97 SJR 1.222 SNIP 0.963
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.115 SNIP 1.066 CiteScore 3.17
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.213 SNIP 1.25 CiteScore 3.36
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.169 SNIP 1.309 CiteScore 2.92
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.329 SNIP 1.281 CiteScore 2.61
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.331 SNIP 1.335 CiteScore 2.74
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.418 SNIP 1.304
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.442 SNIP 1.27
Application of numerical inverse method in calculation of composition-dependent interdiffusion coefficients in finite diffusion couples

The previously developed numerical inverse method was applied to determine the composition-dependent interdiffusion coefficients in single-phase finite diffusion couples. The numerical inverse method was first validated in a fictitious binary finite diffusion couple by pre-assuming four standard sets of interdiffusion coefficients. After that, the numerical inverse method was then adopted in a ternary Al-Cu-Ni finite diffusion couple. Based on the measured composition profiles, the ternary interdiffusion coefficients along the entire diffusion path of the target ternary diffusion couple were obtained by using the numerical inverse approach. The comprehensive comparisons between the computations and the experiments indicate that the numerical inverse method is also applicable to high-throughput determination of the composition-dependent interdiffusion coefficients in finite diffusion couples.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Central South University
Pages: 197-211
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Metallurgical and Materials Engineering
Volume: 23
Issue number: 3
ISSN (Print): 2217-8961
Ratings:
Web of Science (2018): Indexed yes
Application of Photocurrent Model on Polymer Solar Cells Under Forward Bias Stress
We performed a constant current stress at forward bias on organic heterojunction solar cells. We measured current voltage curves in both dark and light at each stress step to calculate the photocurrent. An existing model applied to photocurrent experimental data allows the estimation of several parameters such as generation, recombination, dissociation rate, and nearly zero field voltage within the active layer as a function of the stress time. The analysis of extrapolated parameters shows that the stress mainly affects the recombination rate of the polaron charge transfer states.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Organic Energy Materials, University of Padova
Authors: Rizzo, A. (Ekstern), Torto, L. (Ekstern), Wrachien, N. (Ekstern), Corazza, M. (Intern), Krebs, F. C. (Intern), Gevorgyan, S. (Intern), Cester, A. (Ekstern)
Pages: 1542-1548
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: IEEE Journal of Photovoltaics
Volume: 6
Issue number: 6
ISSN (Print): 2156-3381
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 3.71 SJR 1.214 SNIP 1.447
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.14 SJR 1.513 SNIP 1.569
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.865 SNIP 1.882 CiteScore 4.42
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.196 SNIP 1.806 CiteScore 3.87
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.404 SNIP 3.477 CiteScore 3.84
Scopus rating (2012): SJR 1.014 SNIP 3.11 CiteScore 2.2
Original language: English
Annealing, Current, Heterojunctions, Organic semiconductors, Photovoltaic cells, Roll-to-roll, Solar energy, Stress
Electronic versions:
JPV2016vFinalSubmission.pdf
DOIs:
10.1109/JPHOTOV.2016.2603841
Publication: Research - peer-review › Journal article – Annual report year: 2017

Aqueous metal–organic solutions for YSZ thin film inkjet deposition
Inkjet printing of 8% Y2O3-stabilized ZrO2 (YSZ) thin films is achieved by designing a novel water-based reactive ink for Drop-on-Demand (DoD) inkjet printing. The ink formulation is based on a novel chemical strategy that consists of a combination of metal oxide precursors (zirconium alkoxide and yttrium salt), water and a nucleophilic agent, i.e. n-methyl diethanolamine (MDEA). This chemistry leads to metal–organic complexes with long term ink stability and high
precision printability. Ink rheology and chemical reactivity are analyzed and controlled in terms of metal–organic
interactions in the solutions. Thin dense nanocrystalline YSZ films below 150 nm are obtained by low temperature
calcination treatments (400–500 °C), making the deposition suitable for a large variety of substrates, including silicon,
glass and metals. Thin films and printed patterns achieve full densification with no lateral shrinkage and high ionic
conductivity.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Applied Electrochemistry
, Technical University of Denmark, Ecole Polytechnique Federale de Lausanne (EPFL)
Authors: Gadea, C. (Intern), Hanniet, Q. (Ekstern), Lesch, A. (Ekstern), Marani, D. (Intern), Jensen, S. H. (Intern),
Esposito, V. (Intern)
Pages: 6021-6029
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Materials Chemistry C
Volume: 5
Issue number: 25
ISSN (Print): 2050-7526
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 1.3 SJR 1.917 CiteScore 5.67
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 5.14 SJR 1.825 SNIP 1.266
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.713 SNIP 1.508 CiteScore 5.32
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.517 SNIP 1.351 CiteScore 4.64
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
ISI indexed (2013): ISI indexed no
Original language: English
Electronic versions:
c7tc01879g.pdf
DOIs:
10.1039/C7TC01879G
Publication: Research - peer-review › Journal article – Annual report year: 2017

A regenerative elastocaloric device: Experimental results
Elastocaloric cooling and heating is an alternative cooling technology that has potential to be highly efficient and
environmentally friendly. Experimental results are reported for two elastocaloric regenerators made of NiTi alloys in
the form of parallel plates in two plate thicknesses. For the regenerator made of 0.2 mm plates, a maximum no-load
temperature span of 17.6 K was achieved for an applied strain of 4.3 \%. For the regenerator with 0.35 mm plates, a
maximum temperature span of 19.9 K was reached for a strain of 3.5 \%. The 0.2 mm regenerator failed after
approximately 5200 cycles and the 0.35 mm regenerator failed after approximately 5500 cycles.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, University of Ljubljana,
National Institute of Applied Sciences
Authors: Engelbrecht, K. (Intern), Tusek, J. (Ekstern), Eriksen, D. (Intern), Lei, T. (Intern), Lee, C. (Ekstern), Tušek, J.
(Ekstern), Pryds, N. (Intern)
Number of pages: 21
Publication date: 2017
A simple method for preparing superconducting FeSe pellets without sealing in evacuated silica tubes

Superconducting tetragonal FeSe pellets were made by reacting mixtures of elemental Fe and Se powders in argon atmosphere without sealing in evacuated silica tubes. A simple tube furnace has been used. Although the tube's material consisted of quartz, an alumina tube could be used as well. X-ray pure samples with onset of superconducting transition between 8.0K and 8.5K were obtained under specific heat treatment conditions. Residual, unreacted Fe particles could be virtually eliminated through prolonged annealing. A key factor for the synthesis of good samples consists in using processing parameters that minimize Se losses.
Assembly Modulated by Particle Position and Shape: A New Concept in Self-Assembly

In this communication we outline how the bespoke arrangements and design of micron-sized superparamagnetic shapes provide levers to modulate their assembly under homogeneous magnetic fields. We label this new approach, 'assembly modulated by particle position and shape' (APPS). Specifically, using rectangular lattices of superparamagnetic micron-sized cuboids, we construct distinct microstructures by adjusting lattice pitch and angle of array with respect to a magnetic field. Broadly, we find two modes of assembly: (1) immediate 2D jamming of the cuboids as they rotate to align with the applied field (rotation-induced jamming) and (2) aggregation via translation after their full alignment (dipole-dipole assembly). The boundary between these two assembly pathways is independent on field strength being solely a function of the cuboid's dimensions, lattice pitch, and array angle with respect to field—a relationship which we capture, along with other features of the assembly process, in a 'phase diagram'. In doing so, we set out initial design rules to build custom made assemblies. Moreover, these assemblies can be made flexible thanks to the hinged contacts of their particle building blocks. This flexibility, combined with the superparamagnetic nature of the architectures, renders our assembly method particularly appropriate for the construction of complex actuators at a scale hitherto not possible.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, University Paris Diderot - Paris 7
Authors: Tavacoli, J. W. (Intern), Heuvingh, J. (Ekstern), Du Roure, O. (Ekstern)
Number of pages: 12
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Materials
Volume: 10
Issue number: 11
Article number: 1291
ISSN (Print): 1996-1944
Ratings:
A toolbox to study precious metal nano- catalysts: surfactant free synthesis, characterization and catalytic activity

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Imaging and Structural Analysis, University of Copenhagen, University of Oldenburg, University of Bremen
Authors: Quinson, J. (Forskerdatabase), Simonsen, S. B. (Intern), Kuhn, L. T. (Intern), Kacenauskaite, L. (Ekstern), Inaba, M. (Forskerdatabase), Swane, A. A. (Ekstern), Kirkensgaard, J. J. K. (Ekstern), Jensen, K. Ø. M. (Ekstern), Oezaslan, M. (Ekstern), Kunz, S. (Ekstern), Vosch, T. (Ekstern), Arenz, M. (Ekstern)
Number of pages: 1
Publication date: 2017

Host publication information
Title of host publication: Book of Abstracts Sustain 2017
Article number: C-12
Main Research Area: Technical/natural sciences
Conference: Sustain 2017, Kgs. Lyngby, Denmark, 06/12/2017 - 06/12/2017
Electronic versions:
SustainAbstracts2017c.compressed_27.pdf
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2017

Automated angular and translational tomographic alignment and application to phase-contrast imaging
X-ray computerized tomography (CT) is a 3D imaging technique that makes use of x-ray illumination and image reconstruction techniques to reproduce the internal cross-sections of a sample. Tomographic projection data usually require an initial relative alignment or knowledge of the exact object position and orientation with respect to the detector. As tomographic imaging reaches increasingly better resolution, thermal drifts, mechanical instabilities, and equipment limitations are becoming the main dominant factors contributing to sample positioning uncertainties that will further introduce reconstruction artifacts and limit the attained resolution in the final tomographic reconstruction. Alignment algorithms that require manual interaction impede data analysis with ever-increasing data acquisition rates, supplied by more brilliant sources. We present in this paper an iterative reconstruction algorithm for wrapped phase projection data and an alignment algorithm that automatically takes 5 degrees of freedom, including the possible linear and angular motion errors, into consideration. The presented concepts are applied to simulated and real measured phase-contrast data, exhibiting a possible improvement in the reconstruction resolution. A MATLAB implementation is made publicly available and will allow robust analysis of large volumes of phase-contrast tomography data.
Bismuth phosphates as intermediate temperature proton conductors: From polycrystalline powders to amorphous glasses

Proton conducting electrolyte materials operational in the intermediate temperature range of 200-400 °C are of special interest for applications in fuel cells and water electrolyzers. Bismuth phosphates in forms of polycrystalline powders and amorphous glasses are synthesized and investigated by scanning electron microscopy, X-ray diffraction, FT-IR, thermogravimetric analysis and AC impedance. Under dry atmosphere the pure crystalline and amorphous phosphates exhibit an intrinsic conductivity of up to $10^{-5}$ S cm$^{-1}$ at 250 °C. In the presence of atmospheric humidity the conductivity of both types of phosphates is significantly enhanced, reaching about $10^{-2}$ S cm$^{-1}$ at a water vapor partial pressure above 0.5 atm. During a period of more than 100 h with four humidity cycles from zero to 0.58 atm of the water vapor partial...
pressure, the phosphates show good stability, suggesting the potential as an intermediate temperature electrolyte.
Bottom-Up Design of a Copper-Ruthenium Nanoparticulate Catalyst for Low-Temperature Ammonia Oxidation

A novel nanoparticulate catalyst of copper (Cu) and ruthenium (Ru) was designed for low-temperature ammonia oxidation at near-stoichiometric mixtures using a bottom-up approach. A synergistic effect of the two metals was found. An optimum CuRu catalyst presents a reaction rate threefold higher than that for Ru and forty-fold higher than that for Cu. X-ray absorption spectroscopy suggests that in the most active catalyst Cu forms one or two monolayer thick patches on Ru and the catalysts are less active once 3D Cu islands form. The good performance of the tuned Cu/Ru catalyst is attributed to changes in the electronic structure, and thus the altered adsorption properties of the surface Cu sites.

General information
State: Published
Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics, Center for Electron Nanoscopy, Department of Chemical and Biochemical Engineering, Atomic scale modelling and materials, Universidade de Sao Paulo, Karlsruhe Institute of Technology KIT
Number of pages: 6
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
ISSN (Print): 1433-7851
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): SNIP 2.165 SJR 6.155 CiteScore 11.31
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 10.8 SJR 5.954 SNIP 2.146
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 5.888 SNIP 2.225 CiteScore 11.13
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 5.811 SNIP 2.307 CiteScore 10.84
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 5.702 SNIP 2.198 CiteScore 10.7
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Due to concerns about climate change, negative environmental impacts of some fuels, and the decline in the availability of fossil fuels, renewable energy technologies are growing rapidly and becoming mature. Such technologies can provide a major share of electricity supply demand globally. However, as their market share grows, concerns about potential impacts on the stability and operation of the electricity grid, as well as economic impacts due to grid upgrading requirements, may create barriers to their future expansion, due to renewable electricity’s intermittent productions and variability. ‘Green hydrogen’ can be seen as one of the solutions to integrate high penetrations of renewables in the energy system, using both the electricity and gas networks. At present, the ‘green hydrogen’ market is small and prices are high. However, costs can be driven down by upscaling the production of equipment to mass production; supply chain optimisation, and there is also still room for technology improvement. Now is the time to prepare for the integration of significant quantities of ‘green hydrogen’ into the energy system and gain experience from large-scale demonstration of relevant hydrogen concepts.

The BIG HIT project is creating a replicable hydrogen territory in Orkney (an island archipelago six miles offshore from North of Mainland Scotland) by implementing a fully integrated model of hydrogen production, storage, distribution of the hydrogen across Orkney and utilised for mobility, heat and power. The BIG HIT project will use otherwise curtailed electricity from one wind turbine on Shapinsay and one wind turbine and a tidal test sites on Eday, and use 1.5 MW of Polymer Electrolyte Membrane (PEM) electrolyser to convert it into ~50 t pa of hydrogen. This will be used to provide heat to local public buildings. The excess hydrogen will be transported by ferry in hydrogen tube trailers to the Orkney islands.
largest town, Kirkwall, where it will be used to fuel a 75 kW fuel cell stack (which will provide heat and power to ferries when docked); and the remaining hydrogen will be used at a refuelling station to fuel a fleet of up to 10 electric-hydrogen range extended vans.

The present business model report includes a financial analysis of the demonstration project and should provide an early warning if there is anything that would require the project to be altered (for example, to negotiate negative priced input electricity). By gathering and critically examining inputs from project partners and equipment suppliers: electrolyser (ITM power), tube trailer (Calvera), catalytic hydrogen (H2) boilers (Giacomini), compressor (Hofer), fuel cell stack (Arcola Energy), Hydrogen Fuel Cell (H2 FC) van (SymbioFCell) and other stakeholders, the business model is developed within the 1st year of the project.

The cost analysis of this project considers the life cycle of hydrogen starting from the hydrogen production, transportation, and consumption. The cost includes the fixed cost for equipment and infrastructure investment and operation cost of electricity and water consumption. The functional unit is 1 kg hydrogen produced and consumed. The data collected from the project patterns and suppliers. The current analysis is based on the estimation of hydrogen production and consumption on both Shapinsay and Eday. Another objective of this report is replicability of the concept for follower territories of BIG HIT. So the cost of a replicated BIG HIT concept in the 5th year after starting BIG HIT is modelled based on the assumed capital cost reductions. Capital costs will be driven down through mass production or supply chain optimisation, and also by the technology development.

Under the two different time frames (present expectations and replication after 5 years of BIG HIT), five different scenarios are built to analyse the cost. In the first scenario S1 (current situation with limited use of curtailed energy) and the second scenario S2 (full utilisation of curtailed energy), the electrolysers on Eday and Shapinsay are directly connected to wind turbines and tidal test site. The electricity supply for the electrolyser is only from otherwise curtailed electricity. In the third scenario S3 (full utilisation of electrolysis capacity and the consumed electricity from curtailed electricity), the fourth scenario S4 (full capacity of electrolyser and electricity from both curtailed electricity and power grid), and the fifth scenario S5 (full capacity of electrolyser and the consumed electricity from power grid), the electrolysers are connected to both the wind turbines and tidal test sites and the electricity grid. In the scenarios S3, S4, and S5, it is assumed that the electrolysers can operate at full capacity and run continuously at 24 hours per day. Further it is assumed, that there is a consistent demand of 'green hydrogen' on the market. The difference between the otherwise curtailed electricity and grid electricity is the price. The otherwise curtailed electricity would generate an income from Feed in Tariff (FiT), which also lead to the motivation for the hydrogen producer by using the curtailed electricity. In the current BIG HIT situation (S1) the cost of hydrogen production is calculated to be 9.87 £/kg on Shapinsay and 5.17 £/kg on Eday. Two reasons cause the cost of hydrogen production to be lower on Eday than on Shapinsay. Firstly, hydrogen produced on Eday has the priority to be transported to the fuel cell in Kirkwall, which means there would be no hydrogen unconsumed on Eday. Secondly, the cost of electricity consumed by electrolyser on Eday is less than that on Shapinsay. The difference is made by Eday Renewable Energy Ltd. (ERE) sharing their FiT with the project Surf ‘n’ Turf (SnT) and the BIG HIT project where Shapinsay Renewables Limited, a child company of Shapinsay Development Trust (SDT) does not have the same agreement for the BIG HIT project by now. If the curtailed electricity from the wind turbines could be fully absorbed and the produced hydrogen would be transported and consumed consistently, the cost of producing hydrogen will decrease to 6.92 £/kg on Shapinsay if the agreement of electricity cost is same with that in S1. If the electricity cost is based on FiT, the cost of producing hydrogen will decrease to 2.52 £/kg presented in S2. With increasing of the running capacity, the cost of producing hydrogen can decrease to -2.33 £/kg with FiT support. In the replicated BIT HIT scenarios, the costs of producing hydrogen on Shapinsay are 9.02 £/kg and 2.00 £/kg in S1 and S2, respectively. If there would be no FiT for renewable electricity production in the future, the cost of hydrogen production will be 12.38 £/kg and 13.21 £/kg on Shapinsay and Eday, respectively (S5). The major cost comes from the cost of the electricity consumed from power grid. In the replicated BIT HIT project scenarios, the cost can decrease to 12.34 £/kg and 13.12 £/kg on Shapinsay and on Eday. This difference between from Shapinsay and Eday is due to the different capacity of electrolyser, 1 MW and 0.5 MW respectively.

The utilizations of hydrogen considered in this demonstration project are heat, electricity, and mobility. The replaced conventional energy sources are oil for heat, electricity from power grid, and diesel for mobility. The functional unit is defined as 1 kg hydrogen consumed. The costs of conventional fuels are obtained from the market price. The amounts of conventional fuels are calculated based on the same amounts of energy obtained from 1 kg hydrogen. The considered system boundary includes the hydrogen production process, hydrogen transportation, and hydrogen consumption. At each stage, the data has been collected from the project partners and equipment suppliers/manufacturers. The cost of hydrogen is calculated through the life cycle of hydrogen starting from the hydrogen production, transportation, and consumption. The data collected from the project patterns and suppliers. The current analysis is based on the estimation of hydrogen production and consumption on both Shapinsay and Eday. Another objective of this report is replicability of the concept for follower territories of BIG HIT. So the cost of a replicated BIG HIT concept in the 5th year after starting BIG HIT is modelled based on the assumed capital cost reductions. Capital costs will be driven down through mass production or supply chain optimisation, and also by the technology development.

By the comparison of the total costs for a certain heat, power or mobility service, between hydrogen technologies and conventional technologies, it is concluded that mobility is the application where hydrogen is closest to offer a cost-attractive proposition to the conventional technology, i.e. mobility using diesel as energy source. In the present scenarios, hydrogen is not close to being cost-competitive for neither heat purposes nor power purposes.
Carbazole-based copolymers via direct arylation polymerization (DArP) for Suzuki-convergent polymer solar cell performance

Although direct arylation polymerization (DArP) has recently emerged as an alternative to traditional cross-coupling methods like Suzuki polymerization, the evaluation of DArP polymers in practical applications like polymer solar cells (PSCs) is limited. Because even the presence of minute quantities of defects can dramatically influence the solar cell performance, DArP polymers offer critical insight alongside other structural and optoelectronic comparisons. Even via traditional methods, carbazole-based donors are frequently prone to homocoupling defects, which has been shown to - along with β-defects - compromise performance. Through defect minimization with the bulky and affordable neodecanoic acid (NDA) mixture, we report the synthesis of DArP poly[(9-(heptadecan-9-yl)-9H-carbazole)-alt-(4,7-di(thiophen-2-yl)benzo[c][1,2,5]thiadiazole)] (PCDTBT) that outperforms Suzuki PCDTBT with similar molecular weights. Expanding beyond this model system, carbazole-based polymers featuring 2,5-diethylhexyl-3,6-di(thiophene-2-yl)thiopheno[3,4-c][1,2,5]thiadiazole (TPTl), 5-octyl-1,3-di(thiophen-2-yl)-4H-thieno[3,4-c]pyrrole-4,6(5H)-dione (DT-TPD), and 2,5-bis(2,3-dihydrothieno[3,4-b][1,4]dioxin-5-yl)pyridine (EDOT-Pyr) are generated. Polymers are characterized by 1H NMR, cyclic voltammetry, UV-Vis, GIXRD, SCLC hole mobilities, and are implemented into polymer solar cells fabricated in air under ambient humidity. We demonstrate that DArP polymers perform comparably to Suzuki in practical applications.
Carbon deposition and sulfur poisoning during CO₂ electrolysis in nickel-based solid oxide cell electrodes

Reduction of CO₂ to CO and O₂ in the solid oxide electrolysis cell (SOEC) has the potential to play a crucial role in closing the CO₂ loop. Carbon deposition in nickel-based cells is however fatal and must be considered during CO₂ electrolysis. Here, the effect of operating parameters is investigated systematically using simple current-potential experiments. Due to variations of local conditions, it is shown that higher current density and lower fuel electrode porosity will cause local carbon formation at the electrochemical reaction sites despite operating with a CO outlet concentration outside the thermodynamic carbon formation region. Attempts at mitigating the problem by coating the composite nickel/yttria-stabilized zirconia electrode with carbon-inhibiting nanoparticles and by sulfur passivation proved unsuccessful. Increasing the fuel electrode porosity is shown to mitigate the problem, but only to a certain extent. This work shows that a typical SOEC stack converting CO₂ to CO and O₂ is limited to as little as 15–45% conversion due to risk of carbon formation. Furthermore, cells operated in CO₂-electrolysis mode are poisoned by reactant gases containing ppb-levels of sulfur, in contrast to ppm-levels for operation in fuel cell mode.
Cathode-supported hybrid direct carbon fuel cells

The direct conversion of coal to heat and electricity by a hybrid direct carbon fuel cell (HDCFC) is a highly efficient and cleaner technology than the conventional combustion power plants. HDCFC is defined as a combination of solid oxide fuel cell and molten carbonate fuel cell. This work investigates cathode-supported cells as an alternative configuration for HDCFC, with better catalytic activity and performance. This study aims to define the best processing route to manufacture highly efficient cathode-supported cells based on La0.75Sr0.25MnO3/yttria-stabilized zirconia infiltrated backbones. The challenges on the development of high-performance backbones are discussed. In this study, cathode-supported configuration was confirmed to be more efficient for the oxidation of carbon than anode supported configuration. The maximum power density of the cathode-supported cell increased almost by a factor of two when compared with the anode-supported cell.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Fundamental Electrochemistry

Scopus rating (2014): SJR 1.964 SNIP 2.042 CiteScore 6.3
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.975 SNIP 2.137 CiteScore 5.63
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.282 SNIP 2.006 CiteScore 5.04
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.227 SNIP 2.172 CiteScore 5.13
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 2.294 SNIP 1.972
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 2.105 SNIP 1.785
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.96 SNIP 1.713
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.587 SNIP 1.488
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.802 SNIP 2.223
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.656 SNIP 1.809
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.85 SNIP 1.805
Scopus rating (2003): SJR 1.66 SNIP 1.57
Scopus rating (2002): SJR 2.385 SNIP 1.409
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 1.146 SNIP 1.506
Scopus rating (2000): SJR 0.649 SNIP 0.949
Scopus rating (1999): SJR 0.814 SNIP 0.988

Original language: English
High temperature electrolysis, CO2 reduction, Carbon formation, Sulfur poisoning, Electrode gradients, Mitigation

DOIs: 10.1016/j.jpowsour.2017.10.097
Publication: Research - peer-review › Journal article – Annual report year: 2017
Challenges and Possibilities of EIS on PEMEC

Electrochemical impedance spectroscopy (EIS) has been proven a very strong electrochemical characterization tool in electrochemical research in general and in the areas of fuel cell and battery research in particular. However, this is not the case for polymer electrolyte membrane electrolysis cells (PEMEC), for which relatively few reports on the application of systematic EIS studies are available. Asking experienced researchers in the field about why, the answer has often been that these cells reveal too much electrical noise to obtain EIS with acceptable quality due to O₂ and H₂ bubble formation. Our view of the ideal structure of a PEMEC is that there ought not to be any effect of gas bubbles on the EIS as the current paths should not be disturbed by bubbles. However, we also see noise in our spectra, but the level of noise varies very much from one cell type to another. We have studied noise on three types of PEMEC and two type of alkaline electrolysis cell (AEC) for comparison. A characteristic feature of the studied PEMEC is that there is no or very little noise seen in the EIS in the frequency range above ca. 500 Hz and again not much noise below 5 Hz.

Our hypothesis is that this phenomenon is related to bubbles that are adhering to active sites of the electrocatalyst. When the catalyst layer is subjected to alternating current (AC) during the EIS then, in the PEMEC case, the O₂ pressure and volume of the bubbles growing on the catalyst layer will oscillate with the frequency of the AC. The volume change will naturally change with the frequency. The longer the wave period (the lower the frequency) is, the bigger is the change in the amount of O₂ production during an AC period. In other words, a vibration of the O₂ bubble size and internal pressure must be induced by the AC current. Thus, we imagine that at some low frequency, the bubbles adhering to the catalytic
layer get more unstable and detach with an uneven rate from the catalyst surface. This causes the noise observed. Presumably, the structure and the properties of the interface of the catalyst to the liquid aqueous phase as well as the operation parameter will affect the frequency range and the size of noise in the EIS.

**General information**
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors, Department of Chemistry, EWII Fuel Cells A/S
Authors: Elsøe, K. (Intern), Kraglund, M. R. (Intern), Hjelm, J. (Intern), Jacobsen, T. (Intern), Grahl-Madsen, L. (Ekstern), Mogensen, M. B. (Intern)
Number of pages: 7
Publication date: 2017

**Host publication information**
Title of host publication: Procedings of the 6th European PEFC and Electrolyser Forum 2017
Publisher: European Fuel Cell Forum
Article number: A1002
ISBN (Print): 978-3-905592-22-1
Chapter: 2
Main Research Area: Technical/natural sciences
Conference: 6th European PEFC and Electrolyser Forum 2017, Lucerne, Switzerland, 04/07/2017 - 04/07/2017
Electronic versions:
EFCF_2017_Paper_A1002_Challenge_EIS_PEM_Mogensen_Mogens_05.pdf
Links:
Source: PublicationPreSubmission
Source-ID: 140695070
Publication: Research - peer-review › Article in proceedings – Annual report year: 2017

**Charge transport and structure in semimetallic polymers**
Owing to changes in their chemistry and structure, polymers can be fabricated to demonstrate vastly different electrical conductivities over many orders of magnitude. At the high end of conductivity is the class of conducting polymers, which are ideal candidates for many applications in low-cost electronics. Here, we report the influence of the nature of the doping anion at high doping levels within the semi-metallic conducting polymer poly(3,4-ethylenedioxythiophene) (PEDOT) on its electronic transport properties. Hall effect measurements on a variety of PEDOT samples show that the choice of doping anion can lead to an order of magnitude enhancement in the charge carrier mobility > 3 cm²/Vs at conductivities approaching 3000 S/cm under ambient conditions. Grazing Incidence Wide Angle X-ray Scattering, Density Functional Theory calculations, and Molecular Dynamics simulations indicate that the chosen doping anion modifies the way PEDOT chains stack together. This link between structure and specific anion doping at high doping levels has ramifications for the fabrication of conducting polymer-based devices.

**General information**
State: Published
Organisations: Department of Energy Conversion and Storage, Imaging and Structural Analysis, University of South Australia, Linköping University
Pages: 97-104
Publication date: 2017
Main Research Area: Technical/natural sciences

**Publication information**
Journal: Journal of Polymer Science. Part B, Polymer Physics
Volume: 56
Issue number: 1
ISSN (Print): 0887-6266
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 0.88 SJR 0.837 CiteScore 2.52
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Chemical and Electrochemical Properties of La$_{0.58}$Sr$_{0.4}$Fe$_{0.8}$Co$_{0.2}$O$_{3-\delta}$ (LSCF) Thin Films upon Oxygen Reduction and Evolution Reactions

The Oxygen Evolution and Oxygen Reduction Reactions (OER/ORR), occurring at the oxygen electrode of Solid Oxide Cells (SOCs) in the two possible ways of operation, require substantial overpotentials, therefore lowering the operating efficiency of the cells. The reaction mechanisms occurring at these electrodes are still not completely understood due to
their complexity and localized character at the interfaces between different materials or between the gas atmosphere and
the electrocatalyst, and need in situ techniques with very high chemical sensitivity, with the additional difficulty of probing
the materials as close as possible to their realistic operating conditions. In addition, the properties of LSCF are, despite
numerous studies, still unclear in many aspects, despite LSCF being one of the state-of-the-art electrocatalysts used for
SOCs. It is understood that the surface chemical composition deviates from the nominal bulk composition, and that
secondary phases can segregate at the surfaces and interfaces during operation. Furthermore, the electrochemical
properties such as Area Specific Resistance (ASR), oxygen exchange coefficient ($k_{ex}$), ASR activation energy ($E_a$) and
$pO_2$ exponents for LSCF reported in the literature vary considerably. This study aims to better understand the properties of
LSCF, by combining the results of Electrochemical Impedance Spectroscopy (EIS) and Near-Ambient Pressure X-ray
Photoelectron Spectroscopy (NAP-XPS) on model electrodes, both in polarized and unpolarized conditions. In particular,
NAP-XPS studies of the surface chemistry evolution under operation, as well as the correlation between surface potential
changes in relation to the applied overpotential are addressed, in an attempt to determine the real driving force for the
oxygen reactions. For this purpose, thin films of LSCF are deposited by Pulsed Laser Deposition (PLD) through shadow
masks, in order to obtain well-defined electrode geometries with low risk of contamination, and subsequently tested both in
highly clean EIS measuring setups and at the synchrotron beamline. The results of both kinds of experiments are
correlated, the goal being a better understanding of the material’s properties under operation, as well as possible
degradation phenomena.

**General information**

State: Published

Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry, Department of Chemistry, Stanford University


Publication date: 2017

Event: Abstract from 232nd ECS meeting, National Harbor, Washington, DC, United States.

Main Research Area: Technical/natural sciences

Electronic versions: 10.1007_2Fs00262_017_2001_3_1.pdf

Links: http://ma.ecsdl.org.proxy.findit.dtu.dk/content/MA2017-02/39/1742

Source: FindIt

Source-ID: 2304160858

Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2017

Chemical and Electrochemical Properties of La$_{0.58}$Sr$_{0.4}$Fe$_{0.8}$Co$_{0.2}$O$_{3-δ}$ (LSCF) Thin Films upon Oxygen Reduction and Evolution Reactions

**General information**

State: Published

Organisations: Department of Energy Conversion and Storage, Department of Chemistry, Stanford University


Pages: 1

Publication date: 2017

Conference: 232nd ECS meeting, National Harbor, Washington, DC, United States, 01/10/2017 - 01/10/2017

Main Research Area: Technical/natural sciences

**Publication information**

Journal: Electrochemical Society. Meeting Abstracts (Online)

Volume: MA2017-02

Article number: 1742

ISSN (Print): 2151-2043

Original language: English

Links: http://ma.ecsdl.org.proxy.findit.dtu.dk/content/MA2017-02/39/1742

Publication: Research - peer-review › Conference abstract in journal – Annual report year: 2017

Chemical Production of Graphene Catalysts for Electrochemical Energy Conversion

Recently developed FC technology is among many approaches aiming at solving the global energy challenges. FCs are
electrochemical devices that convert chemical energy from fuel molecules into electrical energy via electrochemical
reactions. FCs are, however, limited by the scarce and expensive platinum (Pt) electrocatalysts. Approach in this Ph.D.
thesis is, therefore, in reducing Pt content to ultra-low loadings in the electrocatalysts and optimizing their electronic
structures to efficiently utilize Pt. Syntheses of small Pt nanoparticles (NPs) were performed in order to increase the
specific area of Pt. Syntheses of core-shell Au-Pt (Au@Pt) NPs, with atomically-thin Pt shells on Au NP cores were
performed. The Au@Pt NPs were further chemically immobilized on a highly conductive graphene support to ensure efficient electronic structure of the catalyst. Graphene possesses unique properties, such as high charge carrier mobility, high conductivity, mechanical strength (130 GPa), and high surface area (2600 m2g-1).[1] Chemical inertness of graphene in polymer electrolyte membrane FC (PEMFC) operating conditions resulted in enhanced electrocatalyst stability. Chemical anchoring of Pt and Au@Pt NPs was achieved via L-cysteine linker molecules that provided pathways for fast electron transfers during the electrocatalytic reactions. Electrochemical properties of self-assembled L-cysteine monolayers immobilized on single-crystal Au(111) surfaces were studied in ionic liquids and their structures imaged by scanning tunneling microscopy (STM), to investigate the nature of L-cysteine bonds on Au. Synthesized electrocatalysts were characterized by spectroscopic, microscopic and electrochemical techniques. Electrocatalysis was examined by electrochemical oxidation of formic acid, methanol and ethanol, and oxygen reduction reaction experiments, for both anode and cathode catalyst applications respectively. Finally, the main goal was to investigate the electrocatalytic performance within the PEMFC systems. Direct formic acid, methanol and ethanol PEMFC station was established. As-synthesized grapheneimmobilized Au@Pt NPs exhibited high electrocatalytic performance and long stability in direct formic acid, methanol and ethanol PEMFCs.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Department of Chemistry
Authors: Seselj, N. (Intern)
Number of pages: 194
Publication date: 2017

Publication information
Place of publication: Kgs. Lyngby
Publisher: DTU Chemistry
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:

Relations
Projects:
Chemical Production of Graphene Catalysts for Electrochemical Energy Conversion
Source: PublicationPreSubmission
Source-ID: 144863705
Publication: Research › Ph.D. thesis – Annual report year: 2018

Chemical solution deposition on textured metal substrates: Enabling sustainability with large-scale and flexible functional thin films

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Imaging and Structural Analysis, Ceramic Engineering & Science
Authors: Grivel, J. (Intern), Thydén, K. T. S. (Intern), Bowen, J. R. (Intern), Bjørnetun Haugen, A. (Intern), Wulff, A. C. (Intern), Yue, Z. (Intern)
Number of pages: 1
Publication date: 2017

Host publication information
Title of host publication: Book of Abstracts, Sustain 2017
Publisher: Technical University of Denmark (DTU)
Article number: M-4
Main Research Area: Technical/natural sciences
Conference: Sustain 2017, Kgs. Lyngby, Denmark, 06/12/2017 - 06/12/2017
Electronic versions:
SustainAbstracts2017c.compressed_118.pdf
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2017

Coarsening of carbon black supported Pt nanoparticles in hydrogen
This study addresses coarsening mechanisms of Pt nanoparticles supported on carbon black in hydrogen. By means of in situ transmission electron microscopy (TEM), Pt nanoparticle coarsening was monitored in 6 mbar 20 % H2/Ar while ramping up the temperature to almost 1000 °C. Time-resolved TEM images directly reveal that separated ca. 3 nm sized Pt nanoparticles in a hydrogen environment are stable up to ca. 800 °C at a heating rate of 10 °C/min. The coarsening above this temperature is dominated by the particle migration and coalescence mechanism. However, for agglomerated Pt
nanoparticles, coalescence events were observed already above 200 °C. The temperature-dependency of particle sizes and the observed migration distances are described and found to be consistent with simple early models for the migration and coalescence.

**General information**
State: Published
Organisations: Department of Energy Conversion and Storage, Imaging and Structural Analysis, Proton conductors, Huaihai Institute of Technology
Authors: Simonsen, S. B. (Intern), Wang, Y. (Ekstern), Jensen, J. O. (Intern), Zhang, W. (Intern)
Number of pages: 9
Publication date: 2017
Main Research Area: Technical/natural sciences

**Publication information**
Journal: Nanotechnology
Volume: 28
Issue number: 47
Article number: 475710
ISSN (Print): 0957-4484
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 3.01 SJR 1.079 SNIP 0.788
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.87 SJR 1.339 SNIP 0.945
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.257 SNIP 1.035 CiteScore 3.07
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.497 SNIP 1.269 CiteScore 3.09
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.602 SNIP 1.231 CiteScore 2.74
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.861 SNIP 1.307 CiteScore 3.34
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.899 SNIP 1.451 CiteScore 3.86
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.844 SNIP 1.252
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.809 SNIP 1.27
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.857 SNIP 1.32
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.899 SNIP 1.348
Web of Science (2007): Indexed yes
Comminution of B₄C powders with a high-energy mill operated in air in dry or wet conditions and its effect on their spark-plasma sinterability

The comminution of a typical submicrometre B₄C powder with a high-energy mill (i.e., a shaker mill) operated in air in either a dry or a wet environment was investigated. It was found that dry shaker milling (i.e., high-energy ball-milling) is able to progressively refine the B₄C particles to the nanoscale. While this is accompanied by oxidation and aggregation, these are not serious drawbacks. Wet shaker milling in methanol (i.e., conventional ball-milling) resulted only in a moderate B₄C particle refinement with greater contamination by the milling tools, which limits its usefulness. It was also found that both dry and wet milling modify the B₄C crystal structure, attributable to carbon enrichment. Consequently, dry shaker milling was found to be more recommendable than wet shaker milling to provide B₄C starting powders with superior sinterability. A comparative densification study by spark-plasma sintering confirmed this recommendation, and also showed the usefulness of dry shaker milling to obtain refined B₄C microstructures for structural applications.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Universidad de Extremadura
Authors: Ortiz, A. L. (Ekstern), Sánchez-Bajo, F. (Ekstern), Leal, V. M. C. (Intern), Guiberteau, F. (Ekstern)
Pages: 3873-3884
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of the European Ceramic Society
Volume: 37
Issue number: 13
ISSN (Print): 0955-2219
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 3.55 SJR 1.068 SNIP 1.698
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.25 SJR 1.142 SNIP 1.888
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.135 SNIP 1.817 CiteScore 3.03
Comparison of iron and copper doped manganese cobalt spinel oxides as protective coatings for solid oxide fuel cell interconnects

MnCo$_2$O$_4$, MnCo$_{1.7}$Cu$_{0.3}$O$_4$, and MnCo$_{1.7}$Fe$_{0.3}$O$_4$ are investigated as coatings for corrosion protection of metallic interconnects in solid oxide fuel cell stacks. Electrophoretic deposition is used to deposit the coatings on Crofer 22 APU alloy. All three coating materials reduce the parabolic oxidation rate in air at 900 °C and 800 °C. At 700 °C there is no significant difference in oxidation rate between coated samples and uncoated pre-oxidized Crofer 22 APU. The cross-scale area specific resistance (ASR) is measured in air at 800 °C using La$_{0.85}$Sr$_{0.1}$Mn$_{1.1}$O$_3$ (LSM) contact plates to simulate the interaction with the cathode in a SOFC stack. All coated samples have three times lower ASR than uncoated Crofer 22 APU after 4370 h aging. The ASR increase with time is lowest with the MnCo$_2$O$_4$ coating, followed by the MnCo$_{1.7}$Fe$_{0.3}$O$_4$ and MnCo$_{1.7}$Cu$_{0.3}$O$_4$ coatings. LSM plates contacted to uncoated Crofer 22 APU contain significant amounts of Cr after aging, while all three coatings effectively prevent Cr diffusion into the LSM. A complex Cr-rich reaction layer develops at the coating-alloy interface during oxidation. Cu and Fe doping reduce the extent of this reaction layer at 900 °C, while at 800 °C the effect of doping is insignificant.
Computational High-throughput Screening for Solar Energy Materials

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Department of Physics, Atomic scale modelling and materials, Theoretical Atomic-scale Physics
Authors: Castelli, I. E. (Intern), Thygesen, K. S. (Intern), Jacobsen, K. W. (Intern)
Number of pages: 30
Publication date: 2017

Host publication information
Title of host publication: Theoretical Modeling of Organohalide Perovskites for Photovoltaic Applications
Publisher: CRC Press
ISBN (Print): 9781498750783
Main Research Area: Technical/natural sciences
Electronic versions:
Publication: Research - peer-review › Book chapter – Annual report year: 2017

Computational Study of Nb-Doped-SnO$_2$/Pt Interfaces: Dopant Segregation, Electronic Transport, and Catalytic Properties
Carbon black, a state-of-the-art cathode material for proton exchange membrane fuel cells (PEMFCs), suffers from severe corrosion in practical applications. Niobium-doped tin dioxide (NTO) is a promising alternative to support the Pt catalysts at the cathodes. Here, through a combined density functional theory and non equilibrium Green's function study, we investigate the Nb segregation at Pt/NTO interfaces under operational electrochemical conditions, and reveal the resulting effects on the electronic transport, as well as the catalytic properties. We find that the Nb dopants tend to aggregate in the subsurface layers of the NTO substrate, whereas their transport across the Pt/NTO interface is hindered by a high thermodynamic barrier under the operating condition of PEMFCs. The interfacial transport of Sn is, however, more facile, indicating possible formations of Sn Pt alloys and tin oxides. The electronic conductivities of the Pt/NTO systems are not
particularly sensitive to the distance of the Nb dopants relative to the interface, but depend explicitly on the Nb concentration and configuration. Through a dopant induced ligand effect, the NTO substrates can improve the catalytic activity of the Pt adsorbate toward the oxygen reduction reaction. We also investigate the co-doped SnO2 substrates by both Nb and Sb elements, and find that a small amount of Nb dopants could further improve the electronic transport of the Pt/Sb-doped-SnO2 interface. The fundamental understanding generated here will help shed light on future applications of Nb-doping and Nb-Sb co-doping in Pt/SnO2 type cathodes for PEMFC applications.
Concentration Impedance in Testing of Solid Oxide Cells Revisited

The concentration impedance originating from diffusion and reactant conversion impedance of the Ni-YSZ supported fuel electrode in solid oxide cell has been treated many times during the latest couple of decades. In spite of this, the separation of the diffusion impedance from the conversion impedance is still not trivial. Therefore, combined theoretical and experimental methods available for breakdown of the concentration impedance are outlined and discussed.
Conductive, transparent and low emissivity coatings of aluminum doped zinc oxide produced by magnetron sputtering

General information
State: Published
Organisations: Department of Energy Conversion and Storage
Authors: Stamate, E. (Intern)
Number of pages: 2
Publication date: 2017

Host publication information
Title of host publication: Proceedings of the 9th International Symposium on Advanced Plasma Science and its Applications for Nitrides and Nanomaterials (ISPlasma2017)
Main Research Area: Technical/natural sciences
Conference: 9th International Symposium on Advanced Plasma Science and its Applications for Nitrides and Nanomaterials (ISPlasma2017), Aichi, Japan, 01/03/2017 - 01/03/2017
Electronic versions:
KS_INV_ISPlasma2017_Invited_Abstract_Stamate_final.pdf
Source: PublicationPreSubmission
Source-ID: 142691279
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2018

Cone-Shaped Gd_{1-x}Sr_xFe_{0.8}Co_{0.2}O_{3-δ} Electrodes for SOFC Cathodes
Five Gd_{1-x}Sr_xFe_{0.8}Co_{0.2}O_{3-δ} perovskites were synthesized using the glycine-nitrate process. The compounds were evaluated as solid oxide fuel cell cathodes using cone-shaped electrodes and electrochemical impedance spectroscopy. It was shown that the electrochemical activity depended on the amount of strontium in the perovskite; the main difference
seemed to be whether the perovskite is a single or a two-phase compound. However, high-strontium-substituted Fe-Co-based perovskites have slightly higher performances than the low-strontium-substituted Fe-Co-based perovskites, as determined by electrochemical impedance spectroscopy on cone-shaped electrodes.

**Conjugated Polymers Via Direct Arylation Polymerization in Continuous Flow: Minimizing the Cost and Batch-to-Batch Variations for High-Throughput Energy Conversion**

Continuous flow methods are utilized in conjunction with direct arylation polymerization (DArP) for the scaled synthesis of the roll-to-roll compatible polymer, poly[(2,5-bis(2-hexyloxy)phenylene)-alt-(4,7-di(thiophen-2-yl)benzo[c][1,2,5]thiadiazole)] (PPDTBT). PPDTBT is based on simple, inexpensive, and scalable monomers using thiényl-flanked benzothiadiazole as the acceptor, which is the first β-protected substrate to be used in continuous flow via DArP, enabling critical evaluation of the suitability of this emerging synthetic method for minimizing defects and for the scaled synthesis of high-performance materials. To demonstrate the usefulness of the method, DArP-prepared PPDTBT via continuous flow synthesis is employed for the preparation of indium tin oxide (ITO)-free and flexible roll-coated solar cells to achieve a power conversion efficiency of 3.5% for 1 cm² devices, which is comparable to the performance of PPDTBT polymerized through Stille cross coupling. These efforts demonstrate the distinct advantages of the continuous flow protocol with DArP avoiding use of toxic tin chemicals, reducing the associated costs of polymer upscaling, and minimizing batch-to-batch variations for high-quality material.
Continuous Hydrothermal Flow Synthesis of Functional Oxide Nanomaterials for Energy Conversion Devices

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors
Authors: Xu, Y. (Intern), Zielke, P. (Intern), Kiebach, W. (Intern)
Number of pages: 1
Publication date: 2017

Host publication information
Title of host publication: Book of Abstracts, Sustain 2017
Publisher: Technical University of Denmark (DTU)
Article number: M-3
Main Research Area: Technical/natural sciences
Conference: Sustain 2017, Kgs. Lyngby, Denmark, 06/12/2017 - 06/12/2017

Continuous Hydrothermal Flow Synthesis of Functional Oxide Nanomaterials Used in Energy Conversion Devices
Continuous hydrothermal flow synthesis (CHFS) was used to prepare functional oxide nanoparticles. Materials synthesized include NiO, Y-doped ZrO2, Gd-doped CeO2, LaCrO3 and Ni-substituted CoFe2O4. These types of oxides can be applied in several energy conversion devices, e.g. as active materials in solid oxide fuel cells (SOFCs), oxygen transport membranes (OTMs), and water electrolysis processes. Compared with other chemical synthesis methods, CHFS is advantageous for preparing nanosized materials with a narrow size distribution and a high phase purity. Moreover, CHFS has a high throughput as materials are continuously produced, and the technology can be scaled-up to an industrial-relevant production capacity.

The thesis starts with investigating the most appropriate mixer design for a novel two-stage reactor by computational fluid dynamics modelling. On basis of the modelling results, a two-stage CHFS reactor was constructed, and proof-of-concept syntheses of NiO and Y-doped ZrO2 (YSZ), in both one-stage and two-stage modes, were conducted. Secondly, Gd-doped CeO2 (GDC) nanoparticles (6 – 40 nm) were synthesized, and the effect of the pH on their size, morphology and composition was studied. An up-scaled synthesis of Gd0.2Ce0.8O2-δ nanoparticles was made, and the as-synthesized particles were processed into inks that displayed a good printability in inkjet printing of electrolytes on both green NiO-GDC and pre-sintered NiO-YSZ substrates. Particularly on the pre-sintered NiO-YSZ substrate, dense continuous layers (< 2 μm in thickness) composed of GDC and YSZ that fully covered the substrate were obtained after firing at 1300 °C.

In addition, (La0.6Sr0.4)0.99CoO3 – Gd0.2Ce0.8O2-δ (LSC-GDC) core-shell type particles were prepared and their high-temperature microstructural evolution was studied in two different sintering processes, i.e. spark plasma sintering and conventional sintering. By conventional hydrothermal batch-type synthesis, a core-shell structure was realized by precipitating ~6 nm large GDC particles on the surface of LSC particles under a mild hydrothermal condition of 100 °C resulting in an integral GDC shell around the LSC core. It was found that by spark plasma sintering, a fine microstructure containing nanograins could be obtained and the graded core-shell architecture could be partially maintained.

For the first time, phase-pure LaCrO3 was obtained by CHFS without any post treatments. A continuous production of cube-shaped LaCrO3 particles (639 nm) was achieved. Processing parameters (temperature and alkali concentration) were found to affect the phase purity of the obtained particles significantly. The synthesized LaCrO3 particles were used to prepare 10Sc1YSZ – LaCrO3 dual-phase oxygen transport membranes. A density of ~90 % was achieved after firing at 1400 °C, which is below normal sintering temperatures for LaCrO3-based ceramics. Oxygen permeation fluxes up to 5 × 10-8 mol cm-2 s-1 were obtained with a 1 mm thick membrane tested in air/N2 at 900 °C.

Finally, CoFe2O4 and Ni-substituted CoFe2O4 nanoparticles were prepared by CHFS and their catalytic properties were evaluated. The CoFe2O4 was found to be active for catalytic CO oxidation. A 50 % conversion of CO at 223 °C and a complete conversion at 310 °C was reached. By CHFS, Ni-substituted CoFe2O4 nanoparticles with controlled Ni contents were synthesized, and their activity as catalysts for the oxygen evolution reaction (the half reaction of water electrolysis) was evaluated. Whereas no simple correlation between the activity and the Ni content was detected, a remarkable improvement of the activity was observed for the sample with 30 at% (in atomic percent) Ni-substituted CoFe2O4 (Co0.7Ni0.3Fe2O4) compared to all other investigated compositions.
Overall, the thesis demonstrates the versatility of the CHFS route for preparing functional oxides in nano particulate form, and documents the properties of the synthesized materials in a number of specific applications (fuel cells, membranes and catalysis).

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Imaging and Structural Analysis
Authors: Xu, Y. (Intern), Kiebach, W. (Intern), Hendriksen, P. V. (Intern), Norby, P. (Intern), Simonsen, S. B. (Intern)
Number of pages: 236
Publication date: 2017

Publication information
Publisher: Department of Energy Conversion and Storage, Technical University of Denmark
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:

Relations
Projects:
Continuous Hydrothermal Flow Synthesis of Functional Oxide Nanomaterials Used in Energy Conversion Devices
Source: PublicationPreSubmission
Source-ID: 139910855
Publication: Research › Ph.D. thesis – Annual report year: 2017

Controlled atmosphere high-temperature scanning probe microscopy (CAHT-SPM)

General information
State: Published
Organisations: Department of Energy Conversion and Storage
Authors: Hansen, K. V. (Intern)
Pages: 203-223
Publication date: 2017

Host publication information
Title of host publication: Metal Oxide-Based Thin Film Structures: Formation, Characterization and Application of Interface-Based Phenomena
Publisher: Elsevier
ISBN (Print): 978-0-12-811166-6
Chapter: 9
Main Research Area: Technical/natural sciences
DOIs:
10.1016/B978-0-12-811166-6.00009-1
Publication: Research - peer-review › Book chapter – Annual report year: 2017

Controlling the Carrier Density of SrTiO$_3$-Based Heterostructures with Annealing
The conducting interface between the insulating oxides LaAlO$_3$ (LAO) and SrTiO$_3$ (STO) displays numerous physical phenomena that can be tuned by varying the carrier density, which is generally achieved by electrostatic gating or adjustment of growth parameters. Here, it is reported how annealing in oxygen at low temperatures ($T < 300 \degree C$) can be used as a simple route to control the carrier density by several orders of magnitude. The pathway to control the carrier density relies on donor oxidation and is thus applicable to material systems where oxygen vacancies are the dominant source of conductivity. Using STO capped with epitaxial γ-Al$_2$O$_3$ (GAO) or amorphous LAO (a-LAO), the pathways for changing the carrier density in the two STO-based cases are identified where oxygen blocking (GAO) and oxygen permeable (a-LAO) films create interface conductivity from oxygen vacancies located in STO near the interface. For a-LAO/STO, the rate limiting step ($E_a = 0.25 \text{ eV}$) for oxidizing oxygen vacancies is the transportation of oxygen from the atmosphere through the a-LAO film, whereas GAO/STO is limited by oxygen migration inside STO ($E_a = 0.5 \text{ eV}$). Finally, it is showed how the control of the carrier density enables writing of conducting nanostructures in γ-Al$_2$O$_3$/STO by conducting atomic force microscopy.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, University of Copenhagen
Authors: Christensen, D. V. (Intern), von Soosten, M. (Intern), Trier, F. (Intern), Sand Jespersen, T. (Ekstern), Smith, A. (Intern), Chen, Y. (Intern), Pryds, N. (Intern)
Correction: Large-scale electricity storage utilizing reversible solid oxide cells combined with underground storage of CO$_2$ and CH$_4$

Correction for 'Large-scale electricity storage utilizing reversible solid oxide cells combined with underground storage of CO$_2$ and CH$_4$' by S. H. Jensen et al., Energy Environ. Sci., 2015, 8, 2471–2479.

General information
State: Published
Authors: Jensen, S. H. (Intern), Graves, C. R. (Intern), Mogensen, M. B. (Intern), Wendel, C. (Ekstern), Braun, R. J. (Ekstern), Hughes, G. (Ekstern), Gao, Z. (Ekstern), Barnett, S. A. (Ekstern)
Number of pages: 1
Pages: 641
Publication date: 2017
Main Research Area: Technical/natural sciences
Corrigendum to “Model for solid oxide fuel cell cathodes prepared by infiltration” [Electrochim. Acta 229 (March (1)) (2017) 73-95]
Authors regret to inform that there was an error in Fig. 4 (equivalent circuit) of the manuscript. The correct equivalent circuit is shown below.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors
Authors: Samson, A. J. (Intern), Søgaard, M. (Intern), Hendriksen, P. V. (Intern)
Pages: 220
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Electrochimica Acta
Volume: 256
ISSN (Print): 0013-4686
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 5.01 SJR 1.439 SNIP 1.101
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
To address sustainability challenges, photovoltaics (PV) are regarded as a promising renewable energy technology. Decreasing PV module costs and increasing residential electricity prices have made self-consumption of PV-generated...
electricity financially more attractive than exporting to the grid. Organic photovoltaics (OPV) are an emerging thin-film PV technology that shows promise of greatly improving the environmental and economic performances of PV technologies. Previous studies have estimated the current and future costs of OPV technologies, but the attractiveness of investing in OPV systems has not been evaluated under real market conditions, especially under PV self-consumption schemes. In this study, we investigate the self-consumption of electricity generation from conventional and organic PV systems installed at residential houses in two different countries, Denmark and Greece, under current PV regulatory frameworks. We then focus on modelling and assessing the cost-competitiveness of organic PV technologies based on cost estimations for existing pilot-scale (kW-range), and projected scale-up (100MW) and industrial-scale (100GW) manufacturing capacity levels. Our generic results applying to all PV technologies show that PV systems installed at residential houses in Greece perform economically better than those in Denmark do in terms of self-sufficiency and gross electricity bill savings (i.e. excluding PV costs). Using the two country cases, which present very different settings, we characterise and discuss the influence of three key parameters of the economic performance of PV systems, namely the PV regulatory scheme, the solar irradiation level and the temporal match between the electricity consumption and solar irradiation profiles. Focusing on organic PV systems developed in an industrial-scale cost setting (1.53€/Wp), we find that they deliver significant electricity bill savings for residential houses in Greece (38%) under current conditions, while they may not be sufficiently attractive for residential houses in Denmark (6.5%) due to mainly the different PV regulatory schemes. Based on these findings, we therefore recommend investors interested in renewable energy technologies to pursue scaling up the manufacturing capacity of OPV technologies, as well as assess a large number of countries to identify and prioritise financially attractive settings for PV self-consumption.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Organic Energy Materials, Quantitative Sustainability Assessment, Department of Management Engineering, University of Western Macedonia
Authors: Chatzisideris, M. D. (Intern), Laurent, A. (Intern), Christoforidis, G. C. (Ekstern), Krebs, F. C. (Intern)
Pages: 471-479
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Applied Energy
Volume: 208
ISSN (Print): 0306-2619
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 8.44 SJR 3.162 SNIP 2.765
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 7.78 SJR 3.011 SNIP 2.61
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 2.835 SNIP 2.593 CiteScore 6.4
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 3.158 SNIP 3.218 CiteScore 6.93
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 3.06 SNIP 3.346 CiteScore 6.59
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.778 SNIP 3.076 CiteScore 5.69
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.416 SNIP 2.827 CiteScore 5.5
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
Coupling between creep and redox behavior in nickel - yttria stabilized zirconia observed in-situ by monochromatic neutron imaging

Ni-YSZ (nickel - yttria stabilized zirconia) is a material widely used for electrodes and supports in solid oxide electrochemical cells. The mechanical and electrochemical performance of these layers, and thus the whole cell, depends on their microstructure. During the initial operation of a cell, NiO is reduced to Ni. When this process is conducted under external load, like also present in a stack assembly, significant deformations of NiO/Ni-YSZ composite samples are observed. The observed creep is orders of magnitude larger than the one observed after reduction during operation. This phenomenon is referred to as accelerated creep and is expected to have a significant influence on the microstructure development and stress field present in the Ni-YSZ in solid oxide electrochemical cells (SOCs), which is highly important for the durability of the SOC. In this work we present energy selective neutron imaging studies of the accelerated creep phenomenon in Ni/NiO-YSZ composite during reduction and also during oxidation. This approach allowed us to observe the phase transition and the creep behavior simultaneously in-situ under SOC operation-like conditions.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Imaging and Structural Analysis, Mixed Conductors, Proton conductors, Xnovo Technology ApS, Paul Scherrer Institut, European Spallation Source ESS AB
Authors: Makowska, M. G. (Intern), Kuhn, L. T. (Intern), Frandsen, H. L. (Intern), Lauridsen, E. M. (Ekstern), De Angelis, S. (Intern), Cleemann, L. N. (Intern), Morgano, M. (Ekstern), Trtik, P. (Ekstern), Strobl, M. (Ekstern)
Pages: 167-175
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Power Sources
Volume: 340
ISSN (Print): 0378-7753
Ratings:
BFI (2018): BFI-level 1
Decisive Intermediates Responsible for the Carbonaceous Products of CO₂ Electro-reduction on Nitrogen-Doped sp² Nanocarbon Catalysts in NaHCO₃ Aqueous Electrolyte

Nitrogen-doped sp² nanocarbon materials have been considered promising catalysts for CO₂ electro-reduction. However, a fundamental understanding about product selectivity and the reaction routes is still lacking. In this report, the reaction mechanism on nitrogen-doped sp² nanocarbon materials is resolved by clarifying the authentic origin of the carbonaceous products: CO and HCO₂⁻. Two carbon-reduction pathways are identified based on a series of comparative studies by using differential electrochemical mass spectrometry and in situ CO adsorption experiments: a dominant pathway leading to CO from CO₂ and a secondary pathway leading to HCO₂⁻ from HCO₃⁻. Neither hydrocarbon (CₓHᵧ) nor alcohol or aldehyde (CₓHᵧOz) were detected in the reduction of CO₂. However, CO, which is generally regarded as an intermediate to be transformed into these products on metal catalysts, can undoubtedly be produced and adsorbed on nitrogen-doped sp² nanocarbon catalysts during the reaction.
Design, enhanced Thermal and Flow efficiency of a 2KW active magnetic regenerator

The goal of the Danish ENOVHEAT project is to design and realize a high-efficiency magnetocaloric heat pump for the residential sector, based on the active magnetic regenerator (AMR) technology. Such a heat pump should have a coefficient of performance (COP) of at least 5, while giving a heating power of 1500 W over a temperature span of 25 K. This paper explains several details of the device, such as the design of the magnet, the regenerator housing and the flow system. In particular, this paper investigates the best geometry for the regenerator bed to achieve a thermal and mechanically efficient housing to be used in the AMR system. Particular attention has been given to the reduction of the parasitic losses through the regenerator housing; both heat leaks between the magnetocaloric material (MCM) and an adjacent iron ring and the surroundings through a lid on top of the regenerator. These quantities have been decreased by creating an embossment on the bottom surface of the regenerator and by placing a thin rubber sheet between the magnetocaloric material and the steel lid, respectively.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Number of pages: 10
Publication date: 2017
Main Research Area: Technical/natural sciences
Magnetic refrigeration, Active magnetic regeneration, Regenerator housing geometry, Heat transfer
Source: PublicationPreSubmission
Source-ID: 137616391
Publication: Research - peer-review › Paper – Annual report year: 2017

Design of oxide electrocatalysts for efficient conversion of CO2 into liquid fuels

Electrochemical conversion of CO2 into high energy density liquid fuels utilizing renewable electricity can usher in a carbon neutral society without limiting the energy consumption. Lack of active and efficient electrocatalysts for this reaction remains a challenge. Research efforts towards catalyst development have obtained limited success due to adsorbate scaling relations on metallic surfaces. Preliminary experimental results indicate rutile oxide catalysts are active at very low overpotential, although the scientific understanding is missing. This thesis aims at delivering knowledge of atomic scale reaction thermodynamic needed to engineer efficient and active oxide electrocatalysts.

Rutile oxides are explored for CO2 reduction reaction (CO2RR) through density functional theory based simulation of reaction thermodynamics. Oxygen atom coordinated intermediates constitute the reaction mechanism active on such catalysts, annulling the scaling laws that limit metallic catalysts. Utilizing model rutile oxide surfaces, trends and limitations of CO2RR on oxide catalysts are analyzed. OH* binding energy is established as the descriptor for CO2RR activity on oxide surfaces. Scaling law based thermodynamic volcano relation for CO2RR is constructed. Guidelines for H* and OH* binding energy range for good activity and selectivity of oxide CO2RR catalysts is proposed. This provides guidance to future development of oxide CO2RR catalysts.

The key role of CO* spectators on reaction onset potential and product selectivity of RuO2 electrocatalyst is elucidated through simulations of CO2RR pathway with varying CO* coverage level. The effect of adsorbate-adsorbate interaction in CO2RR activity is significant. Steric effects from spectator coverage also play a role by altering binding geometry of adsorbates. It is concluded that under experimental condition, CO* coverage is necessary for methanol evolution from RuO2 electrocatalyst, but very high coverage lead to evolution of formic acid and hydrogen together.

Building on the understanding of descriptors for CO2RR activity and CO* spectator effects, a new method of further enhancing the oxide electrocatalyst activity is proposed utilizing ligand effects in mixed oxide systems. Such effects in CO2RR catalysts can produce striking behaviours for adsorbate binding and catalytic properties. Detailed study of such properties for Ru/Ir mixed oxide surfaces with varying metal atom composition as well as different CO* coverages is done. It is identified that monolayer or lesser amount of iridium oxide on RuO2 catalyst can have a methanol onset potential of -0.2 V below RHE. This is attributed to a combination of ligand effect and adsorbate interaction. Through thermodynamic and kinetic barrier calculations, the possibility of 2C products is explored.
Determination of the bonding strength in solid oxide fuel cells' interfaces by Schwickerath crack initiation test

An adaptation of the Schwickerath crack initiation test (ISO 9693) was used to determine the bonding strength between an anode support and three different cathodes with a solid oxide fuel cell interconnect. Interfacial elemental characterization of the interfaces was carried out by SEM/EDS analysis on fracture surfaces to investigate the bonding mechanisms. SEM/EDS of fresh fractures were also performed to determine the cohesion/adhesion mechanism of bonding. Calculations of the residual stresses were determined by finite element simulation using ANSYS, based on thermo-mechanical properties of the materials obtained by measurement, calculation or literature.

General information
State: Published
Organisations: Mixed Conductors, Department of Energy Conversion and Storage, Brno University of Technology, Academy of Sciences of the Czech Republic, University of Modena and Reggio Emilia
Authors: Boccaccini, D. N. (Intern), Sevecek, O. (Ekstern), Frandsen, H. L. (Intern), Dlouhy, I. (Ekstern), Molin, S. (Intern), Charlas, B. (Intern), Hjelm, J. (Intern), Cannio, M. (Ekstern), Hendriksen, P. V. (Intern)
Pages: 3565-3578
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of the European Ceramic Society
Volume: 37
Issue number: 11
ISSN (Print): 0955-2219
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 3.55 SJR 1.068 SNIP 1.698
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.25 SJR 1.142 SNIP 1.888
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.135 SNIP 1.817 CiteScore 3.03
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.163 SNIP 2.083 CiteScore 3.16
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.111 SNIP 1.79 CiteScore 2.57
Determination of the Resistance of Cone-Shaped Solid Electrodes

A cone-shaped electrode pressed into an electrolyte can with advantage be utilized to characterize the electro-catalytic properties of the electrode, because it is less dependent on the electrode microstructure than e.g. thin porous composite electrodes, and reactions with the electrolyte occurring during processing can be avoided. Newman's formula for current constriction in the electrolyte is then used to deduce the active contact area based on the ohmic resistance of the cell, and from this the specific electro-catalytic activity. However, for electrode materials with low electrical conductivity (like Ce$_{1-x}$Pr$_x$O$_{2-δ}$), the resistance of the cell is significantly influenced by the ohmic resistance of the cone electrode, wherefore it must be included. In this work the ohmic resistance of a cone is modelled analytically based on simplified geometries. The two analytical models only differ by a model specific pre-factor, which is consequently determined by a finite element model. The model was applied to measurements on cones of Ce$_{1-x}$Pr$_x$O$_{2-δ}$ characterized on a YSZ electrolyte. Conclusively, the finite element model was used to obtain a formula for the resistance for different cone angles with a small contact area. This reproduces Newman's formula for a cone angle equal to 90°, i.e. a semi-infinite body.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Applied Electrochemistry
Authors: Frandsen, H. L. (Intern), Hendriksen, P. V. (Intern), Koch, S. (Intern), Kammer Hansen, K. (Intern)
Pages: E3035-E3039
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of The Electrochemical Society
Volume: 164
Issue number: 11
ISSN (Print): 0013-4651
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 3.48 SJR 1.267 SNIP 1.009
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.97 SJR 1.222 SNIP 0.963
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.115 SNIP 1.066 CiteScore 3.17
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.213 SNIP 1.25 CiteScore 3.36
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.169 SNIP 1.309 CiteScore 2.92
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.329 SNIP 1.281 CiteScore 2.61
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.331 SNIP 1.335 CiteScore 2.74
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.418 SNIP 1.304
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.442 SNIP 1.27
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.595 SNIP 1.41
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.569 SNIP 1.322
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.608 SNIP 1.535
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.523 SNIP 1.481
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.712 SNIP 1.7
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.971 SNIP 1.677
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 2.036 SNIP 1.618
Web of Science (2002): Indexed yes
Development of Dual-Phase Oxygen Transport Membranes for Carbon Capture Processes

Fossil fuel based power plants and industrial production of cement and steel are major sources of anthropogenic CO₂ emissions. One of the most promising approaches to capture and store CO₂ from such large point sources is the oxy-fuel combustion route, where pure oxygen instead of air is used in the combustion, which greatly facilitates the down-stream CO₂ capture. The main energy penalty for the oxy-fuel process is related to the production of the oxygen, which today commonly is done in cryogenic air separation units (ASUs). An alternative approach, which requires significant less energy is the use of oxygen transport membranes (OTMs), which has the potential to reduce the cost and energy penalty associated with the CO₂ capture and storage.

This thesis focusses on the development and characterization of highly efficient and chemically stable planar asymmetric OTMs for direct integration in oxy-fuel combustion power plants. For the case of direct integration considered here the permeate side of the OTMs will be swept with recirculated flue gas whereby a driving force for oxygen transport through the membrane, which is fed with air on the other side, is directly established. It further facilitates thermal integration and thermal management in the combustion and avoids the need to handle pure oxygen. However, a direct integration scheme impose quite severe conditions on the membrane materials, such as stability towards both CO₂ and SO₂ and at low pO₂ (1-10 mbar).

The development of planar asymmetric membranes in this work, required the parallel development of (i) stable porous supports, (ii) thin dense membrane layers, (iii) porous catalytic backbones and (iv) meso-porous nano-particulate catalytic coatings. For the dense membrane layers, dual-phase composites consisting of a stable ionic and a stable electronic conductor were used to overcome the stability limitations commonly observed with single-phase membrane materials (e.g. La₁₋ₓSrxCo₁₋₂yFe₁₋₂yO₃₋₂δ (LSCF), Ba₁₋ₓSrxCo₁₋₂yFe₁₋₂yO₃₋₂δ (BSCF)) in CO₂ and SO₂. Three composite materials, \((ZrO₂)_{0.89}(Y₂O₃)_{0.01}(Sc₂O₃)_{0.10} - MnCo₂O₄ (10Sc₁YSZ-MCO)\), \((ZrO₂)_{0.89}(Y₂O₃)_{0.01}(Sc₂O₃)_{0.10} - Al₀.₀₂Zn₀.₉₈O₁.₀₁ (10Sc₁YSZ-AZO)\) and \((ZrO₂)_{0.89}(Y₂O₃)_{0.01}(Sc₂O₃)_{0.10} - LaCr₀.₈₅Cu₀.₁₀Ni₀.₀₅O₃₋₂δ (10Sc₁YSZ-LCCN)\) were prepared and applied in planar dual-phase asymmetric OTMs and finally characterized and tested in clean as well as flue-gas like atmospheres.

The work dedicated to 10Sc₁YSZ-MCO (70-30 vol.%) dual-phase membranes entailed development and characterisation of of at least 1 mm thick asymmetric membranes supported on zirconia supports as well as 0.5 mm thick self-standing membranes. The thin asymmetric membranes were prepared by tape-casting, lamination, and fired in a two-step sintering process in order to obtain fully dense thin membrane layers in a sintering regime that avoids excessive Co and Mn diffusion and/or decomposition of the MCO phase. Long-term stability tests over 1700 h in pure CO₂ and 170 h in oxy-fuel conditions (250 ppm of SO₂, 3 vol.% of H₂O, 5 vol.% of O₂ balanced with CO₂) demonstrated the stability of the composite membranes under relevant application conditions. Oxygen permeation fluxes of 1.41 mLN cm⁻² min⁻¹ and 2.23 mLN cm⁻² min⁻¹ at 940 °C in air/N₂ and O₂/N₂ atmospheres, respectively, were obtained. To further improve the membrane performance, catalytic surface layers were developed and tested by electrochemical impedance spectroscopy (EIS). Oxygen permeation
tests were realized on 10Sc1YSZ-MCO (70-30 vol.%) membranes coated with these porous catalytic layers. The tests demonstrated that layers based on mixed ionic and electronic conducting backbones worked best (e.g. Ce0.8Tb0.2O2-δ (CTO)-NiFe2O4 (NFO) (40-60 vol.%)); increases in the oxygen permeation of about 50 % were observed for membranes coated with a such compared to those based on purely ionically conducting backbones.

10Sc1YSZ-AZO (50-50 vol.%) dual-phase composite membranes were also developed and characterized as thick (1 mm) self-standing membranes and thin (8 μm) supported membranes. The stability of these membranes in gas streams containing CO2, SO2 and H2O was found to be excellent. However, the high volatility of the Zn in the AZO phase under mildly reducing atmospheres makes the fabrication of thin asymmetric membranes challenging. Very limited oxygen permeation fluxes were measured through the 8 μm thick supported membrane (0.16 mL N cm-2 min-1 at 925 °C in air/N2), while 1 mm thick membranes, in which the Zn depleted part was removed by polishing, displayed higher oxygen permeation fluxes (0.33 mL N cm-2 min-1 at 925 °C in air/N2).

Finally, self-supported dual-phase membranes made of 70 vol.% of 10Sc1YSZ and 30 vol.% of LCCN were prepared and characterized (oxygen permeation measurements and stability tests under oxy-fuel conditions). Analyses using several characterization techniques (X-ray diffraction (XRD), X-ray fluorescence (XRF), attenuated total reflection Fourier transform infrared spectroscopy (ATR-FTIR), Raman spectroscopy and scanning electronic microscopy with energy dispersive X-ray spectroscopy (SEM-EDX) underlined the excellent stability of the materials under application relevant atmospheres. Oxygen permeation fluxes of 0.27 mL N cm-2 min-1 and 1.02 mL N cm-2 min-1 were obtained at 950 °C in air/N2 gradient for a 1000 μm thick and a 110 μm thick membrane, respectively. To further improve the oxygen permeation through 10Sc1YSZ-LCCN membranes, thin asymmetric and symmetric supported membranes were developed on 10Sc1YSZ-LCCN (40-60 vol.%) porous structures. Fully dense thin membrane layers (10-60 μm) were obtained, but the porous structures (support and activation layers) became too dense in the co-firing process. Consequently, further research and development is required to realize the full potential of this promising material combination.
allowing an entire new perspective in large-scale PV inspection.

**General information**
**State:** Published

**Organisations:** Department of Energy Conversion and Storage, Organic Energy Materials, Department of Photonics Engineering, Diode Lasers and LED Systems, Coding and Visual Communication, Skive Kommune, Kenergy, SiCon • Silicon and PV consulting, Aalborg University, Sky-Watch A/S


**Number of pages:** 2
**Publication date:** 2017

**Host publication information**
**Title of host publication:** Proceedings of the 44th Ieee Photovoltaic Specialists Conference, Pvsc 2017
**Publisher:** IEEE
**Main Research Area:** Technical/natural sciences

**Conference:** 2017 IEEE 44th Photovoltaic Specialists Conference, Washington D.C., United States, 25/06/2017 - 25/06/2017

**Relations**
**Projects:**
Development of outdoor luminescence imaging for drone-based PV array inspection
Source: FindIt
Source-ID: 2355411135
**Publication:** Research - peer-review › Article in proceedings – Annual report year: 2017

**Development of outdoor luminescence imaging for drone-based PV array inspection**
This work has the goal to examine experimentally PV module imaging methods under natural light conditions, that will be used in a fast, accurate and automatic drone-based inspection system for PV power plants.

**General information**
**State:** Published

**Organisations:** Department of Energy Conversion and Storage, Organic Energy Materials, Department of Photonics Engineering, Diode Lasers and LED Systems, Coding and Visual Communication, Skive Kommune, Kenergy, SiCon • Silicon and PV consulting, Aalborg University, Sky-Watch A/S


**Number of pages:** 1
**Publication date:** 2017
**Event:** Paper presented at 5th international workshop on LED and Solar Applications, Kgs. Lyngby, Denmark.
**Main Research Area:** Technical/natural sciences
**Electronic versions:**
[program_20172.pdf](program_20172.pdf)
**Publication:** Research - peer-review › Paper – Annual report year: 2017

**Development of redox stable, multifunctional substrates for anode supported SOFCs**
Redox stable solid oxide fuel cells are beneficial in many aspects such as tolerance against system failures e.g. fuel cut off and emergency shut down, but also allow for higher fuel utilization, which increases efficiency. State-of-the-art Ni-cermet based anodes suffer from microstructural changes upon redox cycling, while other properties such as catalytic activity for methane reforming and/or water gas shift, thermal conductivity in addition to electronic conductivity for current pickup are highly wanted for SOFC applications.

In order to combine the advantages of a redox stable anode with a multifunctional anode support, the development of a two layer fuel electrode based on a redox stable strontium titanate layer for the electrochemically active layer and a redox stable Ni-YSZ support was pursued. Half-cells with well adhering strontium titanate anode layers on state-of-the-art Ni-YSZ cermet supports have been achieved. Redox tolerance of the half-cell depends could be increased by optimizing the redox stability of the cermet support.

**General information**
**State:** Published
Development of Robust Metal-Supported SOFCs and Stack Components in EU METSAPP Consortium

The potential of MS-SOFCs was demonstrated through the previous EU METSOFC project, which concluded that the development of oxidation resistant novel metal-supported solid oxide fuel cell (MS-SOFC) design and stack is the requirement to advance this technology to the next level. The following EU METSAPP project has been executed with an overall aim of developing advanced metal-supported cells and stacks based on a robust, reliable and up-scalable technology. During the project, oxidation resistant nanostructured anodes based on modified SrTiO3 were developed and integrated into MS-SOFCs to enhance their robustness. In addition, the manufacturing of metal-supported cells with different geometries, scalability of the manufacturing process was demonstrated and more than 200 cells with an area of ~150 cm² were produced. The electrochemical performance of different cell generations was evaluated and best performance and stability combination was observed with doped SrTiO3 based anode designs. Furthermore, numerical models to understand the corrosion behavior of the MS-SOFCs were developed and validated. Finally, the cost effective concept of coated metal interconnects was developed, which resulted in 90% reduction in Cr evaporation, three times lower Cr₂O₃ scale thickness and increased lifetime. The possibility of assembling these cells into two radically different stack designs was demonstrated.
Scopus rating (2016): CiteScore 1.79 SJR 0.495 SNIP 0.603
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.685 SNIP 0.779 CiteScore 2.02
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.615 SNIP 0.792 CiteScore 2.05
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.835 SNIP 0.833 CiteScore 1.99
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.24 SNIP 0.993 CiteScore 2.76
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.639 SNIP 1.247 CiteScore 3.31
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.623 SNIP 1.236
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.36 SNIP 1.108
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.506 SNIP 1.211
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.338 SNIP 1.074
Scopus rating (2006): SJR 1.186 SNIP 1.209
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.449 SNIP 0.496
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.259 SNIP 0.348
Web of Science (2004): Indexed yes
Web of Science (2001): Indexed yes
Original language: English
Electronic versions:
post_print_version_efcf.pdf. Embargo ended: 09/05/2018
DOIs:
10.1002/fuce.201600191

Bibliographical note
Paper presented at the 12th EUROPEAN SOFC & SOE FORUM (EFCF2016), July 5–8, 2016 held in Lucerne, Switzerland. Organized by the European Fuel Cells Forum
Source: FindIt
Source-ID: 2358485461
Publication: Research - peer-review › Journal article – Annual report year: 2017

Direct Carbon Oxidation in Modified Solid Oxide Fuel Cells
Hybrid direct carbon fuel cells employ a classical solid oxide fuel cell together with carbon dispersed in a carbonate melt on the anode side. In a European project, the utilization of various coals has been investigated with and without addition of an oxidation catalyst to the carbon-carbonate slurry or anode layer. The nature of the coal affects both open circuit voltage and power output. Highest OCV and power densities were observed for bituminous coal and by adding manganese oxide or praseodymium-doped ceria to the carbon/carbonate mixture. Comparing the carbon black fueled performance of an anode supported (315 μm anodes) and cathode supported cell (15 μm anode) indicates a superior performance of the
latter. Using un-catalyzed biomass (charcoal) as fuel results in an OCV of 941 mV and a maximum power density of 78 mW/cm² at 755°C similar to the power output of manganese oxide catalyzed bituminous coal (73 mW/cm²).

**General information**

State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Centro Nacional del Hidrogeno
Authors: Deleebeeck, L. (Intern), Gil, V. (Intern), Ippolito, D. (Intern), Campana, R. (Ekstern), Kammer Hansen, K. (Intern) , Holtappels, P. (Intern)
Pages: F333-F337
Publication date: 2017
Main Research Area: Technical/natural sciences

**Publication information**

Journal: Journal of the Electrochemical Society
Volume: 164
Issue number: 4
ISSN (Print): 0013-4651
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 3.48 SJR 1.267 SNIP 1.009
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.97 SJR 1.222 SNIP 0.963
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.115 SNIP 1.066 CiteScore 3.17
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.213 SNIP 1.25 CiteScore 3.36
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.169 SNIP 1.309 CiteScore 2.92
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.329 SNIP 1.281 CiteScore 2.61
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.331 SNIP 1.335 CiteScore 2.74
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.418 SNIP 1.304
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.442 SNIP 1.27
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.595 SNIP 1.41
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.569 SNIP 1.322
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.608 SNIP 1.535
Discovery of high-performance low-cost n-type Mg3Sb2-based thermoelectric materials with multi-valley conduction bands

Widespread application of thermoelectric devices for waste heat recovery requires low-cost high-performance materials. The currently available n-type thermoelectric materials are limited either by their low efficiencies or by being based on expensive, scarce or toxic elements. Here we report a low-cost n-type material, Te-doped Mg3Sb1.5Bi0.5, that exhibits a very high figure of merit zT ranging from 0.56 to 1.65 at 300-725K. Using combined theoretical prediction and experimental validation, we show that the high thermoelectric performance originates from the significantly enhanced power factor because of the multi-valley band behaviour dominated by a unique near-edge conduction band with a sixfold valley degeneracy. This makes Te-doped Mg3Sb1.5Bi0.5 a promising candidate for the low- and intermediate-temperature thermoelectric applications.
Dual phase composites for tubular oxygen transport membranes

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Mixed Conductors
Authors: Martinez Aguilera, L. (Intern), Bjørnetun Haugen, A. (Intern), Kiebach, W. (Intern)
Number of pages: 1
Publication date: 2017

Host publication information
Title of host publication: Book of Abstracts, Sustain 2017
Publisher: Technical University of Denmark (DTU)
Article number: M-18
Main Research Area: Technical/natural sciences
Conference: Sustain 2017, Kgs. Lyngby, Denmark, 06/12/2017 - 06/12/2017
Electronic versions:
SustainAbstracts2017c.compressed_128.pdf
Publication: Research › Conference abstract in proceedings – Annual report year: 2017

Durability Studies of High Temperature PEM Fuel Cells. Operational Parameters, Accelerated Testing and Acid Retention

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors, Danish Power Systems ApS
Authors: Jensen, J. O. (Intern), Søndergaard, T. (Intern), Cleemann, L. N. (Intern), Steenberg, T. (Ekstern), Hjuler, H. A. (Ekstern), Li, Q. (Intern)
Number of pages: 1
Publication date: 2017
Event: Abstract from 6th European PEFC and Electrolyzer Forum, Lucerne, Switzerland.
Main Research Area: Technical/natural sciences
Electronic versions:
HT_PEMFC_durability_Jensen_Jens_Oluf_01.pdf
Source: PublicationPreSubmission
Source-ID: 141975463
Publication: Research › Conference abstract for conference – Annual report year: 2017

Dynamic and Impure Perovskite Structured Metal Oxide Surfaces

General information
Dynamic and Impure Perovskite Structured Metal Oxide Surfaces
Surfaces of LSF and LSCF perovskite model electrodes were investigated using a variety of analytical methods on flat model electrodes that were prepared as either pellets or as thin films on top of YSZ pellets in order to throw more light on the widely discussed segregation of layers and particles on the electrode surfaces. An experimental test of the suggestion that the segregation might happen in the vacuum in the analysis equipment gave a negative result. Formation of particles containing significant amounts of S and Cr from segregation of the trace impurities in the acquired powders were observed, and lead us to a new hypothesis about the differences between flat model electrodes and technical nano-sized composite electrodes.
The effect of CeO2 infiltration into the anode or CeO2 mixed with the carbon-fuel on the performance of a Hybrid Direct Carbon Fuel Cell (HDCFC) was studied through the use of polarization curves and electrochemical impedance spectroscopy. The use CeO2 in both ways helped to increase the cell performance. In particular, mixing CeO2 with carbon represents the best strategy to increase the cell power output, probably due to increased formation of CO.
Effect of coating density on oxidation resistance and Cr vaporization from solid oxide fuel cell interconnects

- Protective action of dense and porous spinel coatings on Crofer 22 APU was compared.
- Reduction and re-oxidation produces denser coatings than heat treating in air only.
- Coating density has minor influence on oxidation resistance at 800 °C in air.
- Dense coating resulted in three times lower Cr evaporation rate than porous coating.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Chalmers University of Technology, Norwegian University of Science and Technology
Authors: Talic, B. (Intern), Falk-Windisch, H. (Ekstern), Venkatachalam, V. (Intern), Hendriksen, P. V. (Intern), Wiik, K. (Ekstern), Lein, H. L. (Ekstern)
Pages: 57-67
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Power Sources
Volume: 354
ISSN (Print): 0378-7753
Ratings:
BFI (2018): BFI-level 1
Effect of Sr-doping of LaMnO3 spacer on modulation-doped two-dimensional electron gases at oxide interfaces

Modulation-doped oxide two-dimensional electron gas formed at the LaMnO3 (LMO) buffered disordered-LaAlO3/SrTiO3 (d-LAO/LMO/STO) heterointerface provides new opportunities for electronics as well as quantum physics. Herein, we studied the dependence of Sr-doping of La1-xSr_xMnO3 (LSMO, x = 0, 1/8, 1/3, ½, and 1) spacer on the transport properties of d-LAO/LSMO/STO in order to determine the effects of the filling of Mn eg subbands as well as the LSMO polarity on the modulation-doping. Upon increasing the LSMO film thickness from 1 unit cell (uc) to 2 uc, a sharp metal to insulator transition of interface conduction was observed, independent of x. The resultant electron mobility is higher than 1900 cm² V⁻¹ s⁻¹ at 2 K, which increases upon decreasing x. The sheet carrier density, on the other hand, is in the range of 6.9 × 10¹² to 1.8 × 10¹³ cm⁻² (0.01 to 0.03 e/uc) and is largely independent on x for all the metallic d-LAO/LSMO (1 uc)/STO interfaces. These results are consistent with the charge transfer induced modulation doping scheme and clarify that the polarity of the buffer layer plays a trivial role on the modulation doping. The negligible tunability of the carrier density could result from the reduction of LSMO during the deposition of disordered LAO or that the energy levels of Mn 3d electrons at the interface of LSMO/STO are hardly varied even when changing the LSMO composition from LMO to SrMnO3.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Technical University of Denmark
Authors: Chen, Y. (Intern), Gan, Y. (Intern), Christensen, D. V. (Intern), Zhang, Y. (Ekstern), Pryds, N. (Intern)
Number of pages: 4
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Applied Physics
Volume: 121
Issue number: 9
Article number: 095305
ISSN (Print): 0021-8979
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 0.953 SJR 0.739 CiteScore 2.03
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.72 SJR 0.906 SNIP 0.977
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.821 SNIP 0.996 CiteScore 1.57
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.039 SNIP 1.197 CiteScore 2.04
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.155 SNIP 1.286 CiteScore 2.24
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.312 SNIP 1.291 CiteScore 2.13
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.374 SNIP 1.3 CiteScore 2.24
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
Effects of Gold Substrates on the Intrinsic and Extrinsic Activity of High-Loading Nickel-Based Oxyhydroxide Oxygen Evolution Catalysts

We systematically investigate the effects of Au substrates on the oxygen evolution activities of cathodically electrodeposited nickel oxyhydroxide (NiOOH), nickel–iron oxyhydroxide (NiFeOOH), and nickel–cerium oxyhydroxide (NiCeOOH) at varying loadings from 0 to 2000 nmol of metal/cm². We determine that the geometric current densities, especially at higher loadings, were greatly enhanced on Au substrates: NiCeOOH/Au reached 10 mA/cm² at 259 mV overpotential, and NiFeOOH/Au achieved 140 mA/cm² at 300 mV overpotential, which were much greater than those of the analogous catalysts on graphitic carbon (GC) substrates. By performing a loading quantification using both inductively coupled plasma optical emission spectrometry and integration of the Ni²⁺/³⁺ redox peak, we show that the enhanced activity is predominantly caused by the stronger physical adhesion of catalysts on Au. Further characterizations using impedance spectroscopy and in situ X-ray absorption spectroscopy revealed that the catalysts on Au exhibited lower film resistances and higher number of electrochemically active metal sites. We attribute this enhanced activity to a more homogeneous electrodeposition on Au, yielding catalyst films with very high geometric current densities on flat substrates. By investigating the mass and site specific activities as a function of loading, we bridge the practical geometric activity to the fundamental intrinsic activity.

General information

State: Published
Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics, Department of Energy Conversion and Storage, Stanford University, SLAC National Accelerator Laboratory
Authors: Chakthranont, P. (Ekstern), Kibsgaard, J. (Intern), Gallo, A. (Ekstern), Park, J. (Ekstern), Mitani, M. (Ekstern), Sokaras, D. (Ekstern), Kroll, T. (Ekstern), Sinclair, R. (Ekstern), Mogensen, M. B. (Intern), Jaramillo, T. F. (Ekstern)
Number of pages: 11
Pages: 5399-5409
Efficient p-n junction-based thermoelectric generator that can operate at extreme temperature conditions

In many industrial processes a large proportion of energy is lost in the form of heat. Thermoelectric generators can convert this waste heat into electricity by means of the Seebeck effect. However, the use of thermoelectric generators in practical applications on an industrial scale is limited in part because electrical, thermal, and mechanical bonding contacts between the semiconductor materials and the metal electrodes in current designs are not capable of withstanding thermal-mechanical stress and alloying of the metal-semiconductor interface when exposed to the high temperatures occurring in many real-world applications. Here we demonstrate a concept for thermoelectric generators that can address this issue by replacing the metallization and electrode bonding on the hot side of the device by a p-n junction between the two semiconductor materials, making the device robust against temperature induced failure. In our proof-of-principle demonstration a p-n junction device made from nanocrystalline silicon is at least comparable in its efficiency and power output to conventional devices of the same material and fabrication process, but with the advantage of sustaining high hot side temperatures and oxidative atmosphere.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Electrofunctional materials, University of Duisburg-Essen, O-Flexx Technologies GmbH
Authors: Chavez, R. (Ekstern), Angst, S. (Ekstern), Hall, J. (Ekstern), Maculewicz, F. (Ekstern), Stoetzel, J. (Ekstern), Wiggers, H. (Ekstern), Le, T. H. (Intern), Van Nong, N. (Intern), Pryds, N. (Intern), Span, G. (Ekstern), Wolf, D. E. (Ekstern), Schmechel, R. (Ekstern), Schierning, G. (Ekstern)
Electric Field-Assisted Pressureless Sintering of Ceramic Protonic Conductors

Gadolinium, yttrium and samarium-doped barium cerate pressed pellets were submitted to flash sintering experiments isothermally in the temperature range 800-1300°C under 200 V cm⁻¹ electric field. The pellets were positioned inside a dilatometer furnace with Pt-Ir electrodes connected either to a power supply or to an impedance analyzer to evaluate the bulk and the grain boundary contributions to the electrical resistivity. Near full density was achieved in the sintered samples. The combined results of dilatometry and impedance measurements in conventionally and flash sintered specimens show substantial improvement of the electrical conductivity. Joule heating is assumed to be the primary effect for sintering. Improved grain-to-grain contact and the removal of depleted chemical species due to Joule heating at the space charge region are proposed, respectively, as the reasons for the decrease of the grain boundary component in the impedance diagrams and the improvement of the bulk electrical conductivity.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Federal University of ABC, Nuclear and Energy Research Institute
Authors: Muccillo, R. (Ekstern), Esposito, V. (Intern), de Florio, D. Z. (Ekstern), Muccillo, E. (Ekstern)
Pages: 111-118
Publication date: 2017
Conference: 232nd ECS meeting, National Harbor, Washington, DC, United States, 01/10/2017 - 01/10/2017
Main Research Area: Technical/natural sciences

Publication information
Journal: E C S Transactions
Volume: 80
Issue number: 9
ISSN (Print): 1938-5862
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 0.44 SJR 0.225 SNIP 0.252
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 0.4 SJR 0.228 SNIP 0.253
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.211 SNIP 0.244 CiteScore 0.36
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.212 SNIP 0.234 CiteScore 0.36
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.192 SNIP 0.231 CiteScore 0.27
ISI indexed (2013): ISI indexed no
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.241 SNIP 0.26 CiteScore 0.29
ISI indexed (2012): ISI indexed no
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.261 SNIP 0.28 CiteScore 0.36
Electric Field-Assisted Pressureless Sintering of Ceramic Protonic Conductors

Gadolinium, yttrium and samarium-doped barium cerate (BCGd, BCY and BCSm, respectively) polycrystalline green pellets were submitted to electric field-assisted pressureless sintering experiments isothermally in the temperature range 800-1200°C under 100-200 V cm⁻¹ electric fields, limiting to 1-5 A the electric current pulse amplitude. The sintering experiments were carried out in ambient atmosphere with the pellets positioned inside a vertical dilatometer furnace with Pt-Ir electrodes connected either to a power supply for applying the electric field or to an impedance analyzer for collecting [-Z''(ω) x Z'(ω)] data to evaluate the bulk and the grain boundary contributions to the electrical resistivity. Near full density was achieved in the sintered samples. The combined results of dilatometry and impedance spectroscopy measurements before and after flash sintering show substantial improvement of the electrical conductivity of flash sintered specimens. Joule heating is assumed to be the primary effect of the electric current pulse through the specimens. Improved grain-to-grain contact and the removal of depleted chemical species due to Joule heating at the space charge region are proposed, respectively, as the reasons for the almost total disappearance of the grain boundary component in the impedance diagrams and the improvement of the bulk electrical conductivity.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Nuclear and Energy Research Institute, Universidade Federal do ABC
Authors: Muccillo, R. (Ekstern), Esposito, V. (Intern), Zanetti De Florio, D. (Ekstern), Muccillo, E. (Ekstern)
Number of pages: 1
Publication date: 2017
Conference: 232nd ECS meeting, National Harbor, Washington, DC, United States, 01/10/2017 - 01/10/2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Electrochemical Society. Meeting Abstracts (Online)
Volume: MA2017-02
Article number: 1727
ISSN (Print): 2151-2043
Original language: English
Links:
http://ma.ecsdl.org/content/MA2017-02/39/1727.abstract

Electrocatalysis caught in the act

General information
State: Published
Organisations: Department of Energy Conversion and Storage
Authors: Traulsen, M. L. (Intern), Drasbæk, D. B. (Intern), Holtappels, P. (Intern)
Number of pages: 1
Publication date: 2017

Host publication information
Title of host publication: Book of Abstracts Sustain 2017
Article number: C-5
Electrocatalytic conversion of biomass-derived chemicals in alkaline electrochemical cell

General information
State: Published
Organisations: Department of Energy Conversion and Storage
Authors: Traulsen, M. L. (Intern), Joya, K. S. (Intern), Chatzichristodoulou, C. (Intern)
Number of pages: 1
Publication date: 2017
Main Research Area: Technical/natural sciences
Electronic versions:
DEF_abstract_TERRA_Marie_Lund_Traulsen_final.pdf
Source: PublicationPreSubmission
Source-ID: 138261393
Publication: Research › Conference abstract for conference – Annual report year: 2017

Electrochemical Characterization of a PEMEC Using Impedance Spectroscopy
In this study, electrochemical impedance spectroscopy (EIS) is applied in combination with cyclic voltammetry (CV) and current density – cell voltage curves (i-V-curves) to investigate the processes contributing to the total impedance of a polymer electrolyte membrane electrolysis cell (PEMEC). i-V-curves were linear above 0.35 A cm⁻² implying ohmic processes to be performance limiting, however the impedance spectra showed three arcs indicating three electrochemical reactions at these conditions not to be purely ohmic, but also to have capacitive properties. A hypothesis that the composite IrOₓ/Nafion anode catalyst layer causes two of these arcs with a constant sum of resistance and current constrictions cause the third arc, is suggested. This hypothesis implies that the total differential cell resistance at current densities above 0.35 A cm⁻² is purely ascribed to protonic resistance in Nafion in this type of PEMEC.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, EWII Fuel Cells A/S
Authors: Elsøe, K. (Intern), Grahl-Madsen, L. (Ekstern), Hjelm, J. (Intern), Scherer, G. (Ekstern), Hjelm, J. (Intern), Mogensen, M. B. (Intern)
Pages: F1419-F1426
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of The Electrochemical Society
Volume: 164
Issue number: 13
ISSN (Print): 0013-4651
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 3.48 SJR 1.267 SNIP 1.009
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.97 SJR 1.222 SNIP 0.963
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.115 SNIP 1.066 CiteScore 3.17
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.213 SNIP 1.25 CiteScore 3.36
Web of Science (2014): Indexed yes
Electrochemical Reduction of CO2 on Compositionally Variant Au-Pt Bimetallic Thin Films

The electrocatalytic reduction of CO2 on Au-Pt bimetallic catalysts with different compositions was evaluated, offering a platform for uncovering the correlation between the catalytic activity and the surface composition of bimetallic electrocatalysts. The Au-Pt alloy films were synthesized by a magnetron sputtering co-deposition technique with tunable composition. It was found that the syngas ratio (CO:H2) on the Au-Pt films is able to be tuned by systematically controlling...
the binary composition. This tunable catalytic selectivity is attributed to the variation of binding strength of COOH and CO intermediates, influenced by the surface electronic structure (d-band center energy) which is linked to the surface composition of the bimetallic films. Notably, a gradual shift of the d-band center away from the Fermi level was observed with increasing Au content, which correspondingly reduces the binding strength of the COOH and CO intermediates, leading to the distinct catalytic activity for the reduction of CO2 on the compositionally variant Au-Pt bimetallic films. In addition, the formation of formic acid in the bimetallic systems at reduced overpotentials and higher yield indicates that synergistic effects can facilitate reaction pathways for products that are not accessible with the individual components.

**General information**

State: Published

Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, Delft University of Technology, Eindhoven University of Technology, Interdisciplinary Nanoscience Center, Aarhus University

Authors: Ma, M. (Ekstern), Hansen, H. A. (Intern), Valenti, M. (Ekstern), Wang, Z. (Forskerdatabase), Cao, A. (Ekstern), Dong, M. (Ekstern), Smith, W. A. (Ekstern)

Pages: 51-57

Publication date: 2017

Main Research Area: Technical/natural sciences

**Publication information**

Journal: Nano Energy
Volume: 42
ISSN (Print): 2211-2855

Ratings:

- BFI (2018): BFI-level 2
- Web of Science (2018): Indexed yes
- BFI (2017): BFI-level 1
- Scopus rating (2017): SNIP 1.905 SJR 5.185 CiteScore 13.08
- Web of Science (2017): Indexed Yes
- BFI (2016): BFI-level 1
- Scopus rating (2016): CiteScore 12.26 SJR 4.745 SNIP 1.942
- Web of Science (2016): Indexed yes
- BFI (2015): BFI-level 1
- Scopus rating (2015): SJR 3.921 SNIP 2.203 CiteScore 11.71
- Web of Science (2015): Indexed yes
- BFI (2014): BFI-level 1
- Scopus rating (2014): SJR 3.558 SNIP 2.323 CiteScore 9.74
- BFI (2013): BFI-level 1
- Scopus rating (2013): SJR 3.156 SNIP 2.205 CiteScore 7.76

Original language: English

Electronic versions:
- TAJA_1_s2.0_S2211285517305827_main.pdf
- 1_s2.0_S2211285517305827_main.pdf

DOIs:
- 10.1016/j.nanoen.2017.09.043

Publication: Research - peer-review › Journal article – Annual report year: 2017

**Electrochemical Reduction of CO2 on Ir$_x$Ru$_{1-x}$O$_2$(110) Surfaces**

High overpotentials and low faradic efficiencies plague metal catalysts for direct conversion of CO$_2$ to methanol and other liquid fuels. RuO$_2$-based electrocatalysts have been observed to evolve methanol at low overpotentials, which has been attributed to an alternative reaction mechanism with oxygen-coordinated intermediates that can circumvent the limitations imposed by the scaling relations on metal catalysts. Here, we introduce an innovative concept of ligand effects in oxide catalysts. Both IrO$_2$ and RuO$_2$ binds OH* and other intermediates from the electrochemical reduction of CO$_2$ (CO$_2$RR) strongly, but the stable and miscible system Ir$_x$Ru$_{1-x}$O$_2$ exhibits anomalous weaker binding energy in the presence of CO* spectators, because of Ru–Ir ligand effects. The weakened adsorbate binding leads to a very low CO$_2$RR onset potential (methanol evolution at −0.2 V RHE). An Ir atom at the bridge site with Ru neighbors binds intermediates such as OH* and OCHO* much weaker, because of synergistic ligand effects and adsorbate–adsorbate interactions. Consequently, a RuO$_2$ surface doped with Ir move close to the top of the predicted CO$_2$RR volcano for oxides, which offers a significant improvement over state-of-the-art electrocatalysts for conversion of CO$_2$ into methanol. Analysis of electronic structure parameters with adsorbate binding energies indicates the ligand effect depletes electrons from the Ir atom and shifts the t$_{2g}$ orbitals. The lack of electron donation from CO* spectators to Ir at the active site cause favorable adsorbate binding.
Electrochemical Study of (La0.6Sr0.4)0.99CoO3-δ Thin Film Microelectrodes

Solid Oxide Fuel/Electrolysis Cells (SOFC/SOEC, collectively termed SOC) are one of the most promising reversible energy conversion/storage technologies. Long term durability is required for such devices to become economically feasible. One approach to make SOCs more durable and at a lower cost is to decrease the operation temperature. However, lowering the operation temperature of SOCs has shown to be challenging due to the difficulty in finding suitable oxygen electrodes which have high catalytic activity for oxygen reduction and fast ionic transport. (La,Sr)CoO3-δ (LSC) is one of the promising cathode materials due to its high electronic and ionic conductivity as well as good catalytic activity for oxygen reduction at intermediate temperatures (500-700 °C). However, LSC is characterized by low chemical stability. Multiple degradation mechanisms are reported for LSC such as zirconate formation due to reactivity with YSZ (electrolyte) at operating temperature, decomposition at low pO2, SrO enrichment of and precipitation at the surface and Cr poisoning. Several studies on the electrochemical properties of oxygen electrode materials are reported in the literature. Most of the studies are performed on porous electrodes with the purpose of having a realistic scenario; however we still lack fundamental understanding of the underlying degradation mechanism. Even though porous electrode studies have provided invaluable information about the degradation of the oxygen electrode, the deconvolution of geometrical effects from the intrinsic properties of the material is very difficult. Therefore, the presented work aims to study the oxygen reduction mechanism using geometrically well-defined dense model electrodes. Gd doped CeO2 (CGO) was deposited on polished single crystals YSZ (100) and on top of the CGO layer was deposited a (La0.6Sr0.4)0.99CoO3-δ (LSC40) using...
pulsed laser deposition (PLD). The thin CGO film (~100 nm) was deposited to avoid any reaction between the YSZ and LSC40 (250 nm). Subsequently, using photolithography and ion beam etching the microelectrode arrays with varying diameters (from 100 µm to 5 µm) were produced. Each sample has 4 macro-electrodes which were used as counter-electrode while performing electrochemical measurements. To observe the effect of temperature on the film microstructure and chemistry one sample was heat treated for 16 hours. SEM images, AFM and ToF-SIMS reveal similar behavior for both heat treated and as-deposited films. ToF-SIMS depth profiling reveals a Sr and Co rich surface compared to the bulk of the LSC40 for both samples. The difference between the two samples are in the distribution of common impurities, such as silica. After the heat treatment, the Si signal is higher in the LSC/CGO and CGO/YSZ interfaces (See Figure 1 a-b). The electrochemical measurements were recorded in a Controlled Atmosphere High Temperature Scanning Probe Microscope (CAHT-SPM) which can reach temperatures up to 850 °C. The impedance spectra reveal a high frequency intercept which is related to the conductivity of the electrolyte, a small arc at high/middle frequencies originating from the electrode electrolyte interface, and finally a low frequency arc which is related to the air electrode interface. The evolution of the impedance spectra with changing temperature, atmosphere, polarization and microelectrode size combined with surface chemical analysis and imaging techniques reveals information about the underlying degradation mechanism of LSC electrodes.

**Embedded plasmonic nanoparticles in high refractive index TiOx matrix for photovoltaics applications**

**Resume:** More frequently high refractive index dielectric matrix are used in thin film photovoltaics as transporting layers with good optical proprieties. Doping such matrix with plasmonic resonant scatterers is a promising way to further increase energy conversion efficiencies by trapping incoming light in ultrathin solar cells. Colloidal plasmonic oligomers are obtained following a cost-effective selfassembly strategy and incorporated in organic based cells produced using spincoating techniques in ambient air conditions. An interesting increase is observed of both external quantum efficiency (EQE) and short-circuit current for solar cells loaded with plasmonic oligomers compared with reference organic cells. Theoretical calculations demonstrate that the wavelength dependent EQE enhancement is a resonant process due to the increased scattering efficiency in plasmonic antennas allowed by a chemically controlled 1 nm nanogap. The nanogap antennas are linked at a controlled distance of a few nanometers by Dithiothreitol molecules. The spacing molecules ensure a minimum distance that plays a fundamental role in the formation of intensity hot spots in the nanogap as well as large and redshifted scattering peaks. This OPV device, realized in ambient air condition, exhibited an efficiency 14% higher than the reference one showing a relevant enhancement in the red part of the EQE measurements.

**General information**

**State:** Published

**Organisations:** Department of Energy Conversion and Storage, Department of Chemistry

**Authors:** Kreka, K. (Intern), Hansen, K. V. (Intern), Jacobsen, T. (Intern), Normann, K. (Intern), Chatzichristodoulou, C. (Intern), Mogensen, M. B. (Intern)

**Publication date:** 2017

**Event:** Abstract from 232nd ECS meeting, National Harbor, Washington, DC, United States.

**Main Research Area:** Technical/natural sciences

**Links:**

http://ma.ecsdl.org.proxy.findit.dtu.dk/content/MA2017-02/39/1726#aff-2

**Source:** FindIt

**Source-ID:** 2304160853

**Publication:** Research - peer-review › Conference abstract for conference – Annual report year: 2017

**Bibliographical note**

SYMPOSIUM R: Nanoparticles in dielectric matrix: from synthesis to device applications for photonics, electronics, and biosensing (abstract R 10.3)

**Source:** PublicationPreSubmission

**Source-ID:** 134441470

**Publication:** Research - peer-review › Conference abstract for conference – Annual report year: 2017
Encapsulated iron-based oxygen reduction electrocatalysts by high pressure pyrolysis

Non-precious metal catalysts (NPMCs) are candidate materials to replace platinum for proton exchange membrane fuel cells (PEMFCs). Herein we reported a type of iron-based NPMCs prepared by high pressure pyrolysis for the oxygen reduction reaction (ORR) in acidic media. The catalysts are in form of carbon microspheres in a sub-microscale consisting of iron-containing nanoparticles encapsulated by graphitic layers. By tailoring temperatures and duration of pyrolysis, the best ORR catalyst was achieved at 700 degrees C and 75 min, which exhibits an onset potential of 0.85 V at 0.1 mA cm(-2) and a half-wave potential of 0.72 V in acid media. After 10,000 potential cycles, only 25 mV shift of half-wave potential is observed showing excellent stability. An analogue material prepared from nitrogen-free precursors shows significant electrochemical activity though it is much lower than that from the nitrogen containing precursors and can be improved by post treatment in ammonia. These results indicate the contribution to the catalysis from surface nitrogen functionalities and encapsulated metal-containing nanoparticles. (C) 2017 Hydrogen Energy Publications LLC. Published by Elsevier Ltd. All rights reserved.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors, Technical University of Denmark
Authors: Zhong, L. (Intern), Hu, Y. (Intern), Cleemann, L. N. (Intern), Pan, C. (Intern), Svaerke, J. (Ekstern), Jensen, J. O. (Intern), Li, Q. (Intern)
Pages: 22887-22896
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Volume: 42
Issue number: 36
ISSN (Print): 0360-3199
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 4.1 SJR 1.116 SNIP 1.267
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.74 SJR 1.145 SNIP 1.315
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.27 SNIP 1.314 CiteScore 3.46
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.207 SNIP 1.484 CiteScore 3.54
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.265 SNIP 1.449 CiteScore 3.38
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.499 SNIP 1.708 CiteScore 3.96
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.443 SNIP 1.828 CiteScore 4.42
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.579 SNIP 1.854
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.32 SNIP 1.87
Energy modelling towards low carbon development of Beijing in 2030

Beijing, as the capital of China, is under the high pressure of climate change and pollution. The consumption of non-renewable energy is one of the most important sources of the CO2 emissions, which cause climate changes. This paper presents a study on the energy system modelling towards renewable energy and low carbon development for the city of Beijing. The analysis of energy system modelling is organized in two steps to explore the alternative renewable energy system in Beijing. Firstly, a reference energy system of Beijing is created based on the available data in 2014. The EnergyPLAN, an energy system analysis tool, is chosen to develop the reference energy model. Secondly, this reference model is used to investigate the alternative energy system for integrating renewable energies. Three scenarios are developed towards the energy system of Beijing in 2030, which are: (i) reference scenario 2030, (ii) BAU (business as usual) scenario 2030, and (iii) RES (renewable energies) scenario 2030. The 100% renewable energy system with zero CO2 emission can be achieved by increasing solar energy, biomass and municipal solid waste (MSW) and optimizing heating system. The primary fuel consumption is reduced to 155.9 TWh in the RES scenario, which is 72% of fuel consumption in the reference scenario 2030.
Municipal activities play an important role in national and global CO2-emission reduction efforts, with Nordic countries at the forefront thanks to their energy planning tradition and high penetration of renewable energy sources. In this work, we present a case study of the Danish municipality of Sønderborg, whose aim is to reach zero net CO2 emissions by 2029. Sønderborg has an official strategic plan towards 2029, which we compared with four alternative scenarios to investigate how the municipality could approach its target in the most energy-efficient and cost-effective way while simultaneously keeping biomass and waste consumption close to the limits of the locally available residual resources. We modelled all sectors of the energy system on the municipal scale, applying a broad range of energy conversion technologies, including
advanced biomass conversion technologies and reversible electrolysis. We constructed five scenarios, each representing a different energy mix for Sønderborg’s energy system in 2029. We modelled these scenarios using the mixed-integer linear optimization tool Sifre. We compared the results for the five scenarios using four indicators: annual total system cost, total energy system efficiency, annual net system CO2 emissions and total annual biomass consumption. The results show that scenarios with a high degree of electrification perform better on the selected indicators than scenarios with a high degree of biomass utilization. Moreover, the incorporation of advanced conversion technologies such as electrolysis, fuel cells and methanol production further reduces both the total system cost and net CO2 of the highly electrified energy system. Our sensitivity analysis demonstrates that scenarios with a low biomass consumption and a high degree of electrification are less dependent on changes in energy prices. We conclude that in order to achieve their CO2 emission goals in the most energy-efficient, cost-effective and sustainable way, municipalities similar to Sønderborg should compare a wide range of energy system configurations, for example, scenarios with a high degree of electrification and a limited biomass use.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Department of Management Engineering, Systems Analysis, Energinet.dk
Authors: Sveinbjörnsson, D. Þ. (Intern), Ben Amer-Allam, S. (Intern), Hansen, A. B. (Ekstern), Algren, L. (Ekstern), Pedersen, A. S. (Intern)
Pages: 922-941
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Applied Energy
Volume: 195
ISSN (Print): 0306-2619
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 8.44 SJR 3.162 SNIP 2.765
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 7.78 SJR 3.011 SNIP 2.61
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 2.835 SNIP 2.593 CiteScore 6.4
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 3.158 SNIP 3.218 CiteScore 6.93
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 3.06 SNIP 3.346 CiteScore 6.59
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.778 SNIP 3.076 CiteScore 5.69
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.416 SNIP 2.827 CiteScore 5.5
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.531 SNIP 2.259
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.992 SNIP 1.85
Enhanced densification of thin tape cast Ceria-Gadolinium Oxide (CGO) layers by rheological optimization of slurries

Optimized CGO-based slurries are formulated and shaped into thin dense layers via a tape-casting process. The formulation is adjusted with respect to the rheological behaviour. The internal structure and flow properties of slurries are explored with the aim of identifying the required conditions to obtain thin dense CGO layers at reduced sintering temperatures (1200 °C). We demonstrate a correlation between the rheological properties of the slurries, the sintering behaviour and the microstructure of the resulting tapes. Remarkably, a dense CGO layer less than 20 μm thick is obtained with a non-congested slurry, having optimized ceramic loading and liquid-like behaviour.
Environmental impacts of electricity self-consumption from organic photovoltaic battery systems at industrial facilities in Denmark

Organic photovoltaics (OPV) show promise of greatly improving the environmental and economic performance of PV compared to conventional silicon. Life cycle assessment studies have assessed the environmental impacts of OPV, but not under a self-consumption scheme for industrial facilities. We investigate the life cycle environmental impacts of electricity self-consumption from an OPV system coupled with a sodium/nickel chloride battery at an iron/metal industry in Denmark. Results show that an OPV system without storage could decrease the carbon footprint of the industry; installation of the battery increases climate change and human toxicity impacts. We discuss sensitive modelling parameters and provide recommendations.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Organic Energy Materials, Quantitative Sustainability Assessment, Transport DTU, Department of Management Engineering
Transportation based on sustainable energy requires an energy carrier, which is able to store the predominately electrical energy generated from sustainable sources in a high energy density form. Metal-air batteries, hydrogen and synthetic fuels are possible future energy carriers. Density functional theory calculations contribute in research and development of these technologies.

Systematic errors are present in calculations with general gradient approximation functionals for all three technologies. Such functionals will in many cases be the best compromise of computational cost and accuracy if not for the systematic errors. In this thesis it is shown how the systematic errors can be mitigated.

For different alkali and alkaline earth metal oxides, systematic errors have previously been observed. These errors are primarily caused by differences in metal element oxidation state. The systematic errors can be significantly reduced by using metal chlorides rather than pure bulk metals as point of reference for metal oxide energies.

Systematic errors in gas phase CO2 reduction reactions have previously been attributed a molecular O-C-O backbone structure. They are through error correlations found to be caused by individual C=O bonds. Energy corrections applied to C=O bonds significantly reduce systematic errors and can be extended to adsorbates.

A similar study is performed for intermediates in the oxygen evolution and oxygen reduction reactions. An identified systematic error on peroxide bonds is found to also be present in the OOH* adsorbate. However, the systematic error will almost be canceled by inclusion of van der Waals energy. The energy difference between key adsorbates is thus similar to that previously found.

Finally, a method is developed for error estimation in computationally inexpensive neural networks. The method can validate the use of a neural network for emulation of density functional theory calculations for given atomic configuration.

**General information**

State: Published  
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials  
Authors: Christensen, R. (Intern), Vegge, T. (Intern), Hansen, H. A. (Intern)  
Number of pages: 210  
Publication date: 2017

**Publication information**

Publisher: Department of Energy Conversion and Storage, Technical University of Denmark  
ISBN (Print): 978-87-92986-58-0  
Original language: English  
Main Research Area: Technical/natural sciences  
Electronic versions:  
PhD_thesis_Rune_Christensen.pdf

**Relations**

Projects:  
Error Mitigation in Computational Design of Sustainable Energy Materials  
Source: PublicationPreSubmission  
Source-ID: 133053113  
Publication: Research › Ph.D. thesis – Annual report year: 2017
Estimation of current constriction losses via 3D tomography reconstructions in electrochemical devices: a case study of a solid oxide cell electrode/electrolyte interface

In the present study, the methodology for accurate estimations of the current constriction resistance in solid state electrochemical devices via 3D tomography reconstructions is developed. The methodology is used to determine the current constriction resistances at the Ni:YSZ anode/YSZ electrolyte interface of a solid oxide fuel cell. The current constriction at this interface becomes increasingly important as thinner electrolyte layers are continuously being pursued for increased performance. Various possible scenarios have been illustrated on idealized geometries as a function of electrolyte thicknesses, from which it is clear, that for a given set of electrodes an optimal electrolyte thickness exist. Thus, increased performance by reduction of the electrolyte thickness is only feasible down to a certain thickness, after which, a lower performance is obtained on a further reduction of the electrolyte thickness. The obtained results on current constriction resistances from numerical calculations on a 3D reconstruction of a Ni:YSZ anode/YSZ electrolyte assembly is compared with existing models with analytical expressions. The comparison shows, that the assumptions of existing models are by far too simple and the models are therefore not applicable for technological relevant electrochemical devices.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry, Imaging and Structural Analysis
Authors: Nielsen, J. (Intern), Jørgensen, P. S. (Intern)
Pages: 387-396
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Electrochimica Acta
Volume: 252
ISSN (Print): 0013-4686
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 5.01 SJR 1.439 SNIP 1.101
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.74 SJR 1.355 SNIP 1.177
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.321 SNIP 1.324 CiteScore 4.86
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.378 SNIP 1.456 CiteScore 4.59
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.427 SNIP 1.587 CiteScore 4.44
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.644 SNIP 1.574 CiteScore 3.99
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.615 SNIP 1.788 CiteScore 4.15
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.685 SNIP 1.715
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.523 SNIP 1.615
Evolution of concentration fluctuation during phase separation of polystyrene/poly (vinyl methyl ether) blend in the presence of nanosilica

The influence of nanosilica on the concentration fluctuation of polystyrene/poly (vinyl methyl ether) (PS/PVME) mixtures was investigated during phase separation. The amplitude of concentration fluctuation was quantified by dielectric spectrums based on the idea of Lodge–Mcleish model and the linearized Cahn–Hilliard theory could describe the amplitude evolution of concentration fluctuation at the early stage of phase separation. Hydrophilic nanosilica A200 dispersed in PVME-rich phase behaved an obvious inhibition effect on the concentration fluctuation of blend matrix, while hydrophobic nanosilica R974 dispersed in PS-rich phase had little effect on the concentration fluctuation. The kinetics and amplitude evolution of concentration fluctuation during phase separation for PS/PVME/A200 nanocomposites were remarkably restrained due to the surface adsorption of PVME on A200. As the segmental dynamics of PVME and PS in homogeneous matrix was hardly influenced by A200 and R974, the enhanced miscibility and the significantly constrained flow relaxation of PVME chains might contribute to the retarded concentration fluctuation of PS/PVME/A200 nanocomposites. While the weak interaction between R974 and components of blend matrix and little effect of R974 on the molecular dynamics of PS chains may result in the weak retardation of concentration fluctuation for blend matrix.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Zhejiang University
Authors: Chen, Q. (Ekstern), Zuo, M. (Ekstern), Yang, R. (Ekstern), Zhang, J. (Ekstern), LV, X. (Ekstern), Zhang, W. (Intern), Song, Y. (Ekstern), Zheng, Q. (Ekstern)
Number of pages: 13
Pages: 1337-1349
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Polymer Science. Part B, Polymer Physics
Volume: 55
Issue number: 17
ISSN (Print): 0887-6266
Ratings:
BFI (2018): BFI-level 1
Experimental Determination of the Formation Enthalpy of Calcium Cobaltate from Sol–Gel Precursors

Calcium cobaltate (Ca₃Co₄O₉) remains one of the most promising p-type oxide materials for high-temperature thermoelectric energy conversion. While much progress has been made in refining our understanding of the unique structure of the material, as well as optimization of the transport properties for thermoelectric efficiency, there remains a gap in the knowledge, both experimental and theoretical, of the thermodynamics of the system. Presented herein is an analysis of the heat of formation of the Ca₃Co₄O₉ phase from sol–gel precursors using a highly sensitive differential
scanning calorimeter, as well as observations of its decomposition into the Ca₃Co₂O₆ phase. The reaction enthalpy of forming Ca₃Co₄O₉ from CaCO₃ and Co₃O₄ sol–gel precursors was determined to be +284 (±2%) kJ/mol, leading to a standard enthalpy of Ca₃Co₄O₉ of −3307 (±3.5%) kJ/mol.

General information
State: Published
Authors: Holgate, T. C. (Ekstern), Wu, N. (Intern), Van Nong, N. (Intern), Pryds, N. (Intern)
Number of pages: 5
Pages: 1413–1417
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Electronic Materials
Volume: 46
Issue number: 2
ISSN (Print): 0361-5235
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SJR 0.474 SNIP 0.772 CiteScore 1.59
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.49 SJR 0.487 SNIP 0.754
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.555 SNIP 0.802 CiteScore 1.53
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.679 SNIP 1.05 CiteScore 1.82
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.71 SNIP 1.094 CiteScore 1.71
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.865 SNIP 1.298 CiteScore 1.74
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.844 SNIP 1.139 CiteScore 1.66
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.773 SNIP 1.035
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.907 SNIP 1.133
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.858 SNIP 0.953
Scopus rating (2007): SJR 0.879 SNIP 1.058
Scopus rating (2006): SJR 1.028 SNIP 1.222
Scopus rating (2005): SJR 1.13 SNIP 1.199
Scopus rating (2004): SJR 1.097 SNIP 1.184
Web of Science (2004): Indexed yes
Ex-situ tracking solid oxide cell electrode microstructural evolution in a redox cycle by high resolution ptychographic nanotomography

For solid oxide fuel and electrolysis cells, precise tracking of 3D microstructural change in the electrodes during operation is considered critical to understand the complex relationship between electrode microstructure and performance. Here, for the first time, we report a significant step towards this aim by visualizing a complete redox cycle in a solid oxide cell (SOC) electrode. The experiment demonstrates synchrotron-based ptychography as a method of imaging SOC electrodes, providing an unprecedented combination of 3D image quality and spatial resolution among non-destructive imaging techniques. Spatially registered 3D reconstructions of the same location in the electrode clearly show the evolution of the microstructure from the pristine state to the oxidized state and to the reduced state. A complete mechanical destruction of the zirconia backbone is observed via grain boundary fracture, the nickel and pore networks undergo major reorganization and the formation of internal voids is observed in the nickel-oxide particles after the oxidation. These observations are discussed in terms of reaction kinetics, electrode mechanical stress and the consequences of redox cycling on electrode performance.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Imaging and Structural Analysis, Paul Scherrer Institut
Authors: De Angelis, S. (Intern), Jørgensen, P. S. (Intern), Esposito, V. (Intern), Hsiao Rho Tsai, E. (Ekstern), Holler, M. (Ekstern), Kreka, K. (Intern), Abdellahi, E. (Intern), Bowen, J. R. (Intern)
Pages: 520-527
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Power Sources
Volume: 360
ISSN (Print): 0378-7753
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 7 SJR 2.202 SNIP 1.536
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 6.22 SJR 1.944 SNIP 1.5
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.9 SNIP 1.667 CiteScore 6.34
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.964 SNIP 2.042 CiteScore 6.3
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.975 SNIP 2.137 CiteScore 5.63
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Fe-Ni Nanoparticles: A Multiscale First-Principles Study to Predict Geometry, Structure, and Catalytic Activity

Nanoparticles of iron and nickel are promising candidates as nanosized soft magnetic materials and as catalysts for carbon nanotube synthesis and CO methanation, among others. To understand geometry- and size-dependent properties of these nanoparticles, phase diagram of Fe/Ni alloy nanoparticles was calculated by density functional theory and cluster expansion method. Ground state convex is presented for FCC, BCC, and icosahedral particles. Previous experimental observations were explained by using multiscale model for particles with realistic size (diameter ≥ 2 nm). At size 1.5 nm, geometry changes from BCC at low X(Ni) to icosahedral at high X(Ni). FCC is stabilized over icosahedral geometry by increasing number of atoms from 561 to 923. In large FCC particles, there is enrichment of Fe atoms from core to shell beneath surface, while surface and core are enriched by Ni atoms. Catalytic enhancement effect in CO methanation was found to be due to Ni incorporating in the active sites which brings adsorption energy of oxygen closer to the optimum. The predicted phase diagrams and implications on catalysis are expected to help rationalisation of experimental results and provide guidance for design of Fe/Ni-based nanomaterials.
Ferromagnetic Two-Dimensional Electron Gases at the Interface between Two Oxide Insulators

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Authors: Chen, Y. (Intern)
Number of pages: 1
Publication date: 2017
Main Research Area: Technical/natural sciences
Electronic versions:
Abstract_Yunzhong_DTU_Ferromagnetic_Two_Dimensional_Electron_Gases_at_the_Interface_between_Two_Oxide_Insulators.pdf
Source: PublicationPreSubmission
Source-ID: 140347258
Publication: Research › Conference abstract for conference – Annual report year: 2017

From 3D to 2D Co and Ni Oxyhydroxide Catalysts: Elucidation of the Active Site and Influence of Doping on the Oxygen Evolution Activity

Layered oxyhydroxides (ox-hys) of Ni and Co are among the most active catalysts for oxygen evolution in alkaline media. Their activities can be further tuned by delamination into single-layer oxide sheets or by means of doping. The active site for the reaction and how doping and delamination promote the intrinsic activity, however, remain elusive. To shed light on these open questions, we have undertaken a systematic analysis of the stability, catalytic activity, and electronic conductivity of Ni and Co ox-hys ranging from bulk (3D) to single-layer (2D) catalysts. In both cases, we investigate the role of terrace and edge sites and use stability, catalytic activity, and electronic conductivity as evaluation criteria to pinpoint the best catalysts. We arrive at several important conclusions: the ox-hy surface is fully oxidized under oxygen evolution conditions, bulk terraces are ostensibly the most active sites, and Ni ox-hy sheets are more electronically conductive in comparison to their Co equivalents. Furthermore, we examine 25 different doped Co and Ni ox-hy nanosheets (V, Cr, Mn, Fe, Co/Ni, Cu, Ru, Rh, Pd, Ir, Pt, Ag, Al, Ga, In, Sn, Pb, Bi, Mg, Sc, Y, Ti, Nb, Zn, and Cd) to further tailor the catalytic performance. We establish the dependence of the electronic conductivity and activity on potential and find that it is more energetically favorable to dope Ni in comparison to Co ox-hys, with first-row transition and noble metals being the most stable dopants. Finally, we extend the analysis to include bulk terminations and reveal that most dopants, which are stable in the nanosheets, have a large propensity to segregate to the surface of bulk materials, and those that are less prone to segregation (Fe or Cr) are not electronically conductive in the bulk. Overall, we identify Rh-doped Ni ox-hy to be the best catalyst material.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials
Authors: Tripkovic, V. (Intern), Hansen, H. A. (Intern), Vegge, T. (Intern)
Pages: 8558-8571
Publication date: 2017
Main Research Area: Technical/natural sciences
Publication information
Journal: A C S Catalysis
Volume: 7
Issue number: 12
ISSN (Print): 2155-5435
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 11.49 SJR 4.921 SNIP 2.113
Web of Science (2017): Indexed yes
Gel Electrolytes of Covalent Network Polybenzimidazole and Phosphoric Acid by Direct Casting
Polybenzimidazole membranes imbibed with phosphoric acid can support high proton conductivity at 120–200 °C, and have therefore emerged as the state-of-the-art electrolytes for fuel cells operating in this temperature range. This work presents a novel and operationally simple methodology for preparing mechanically robust covalent network polybenzimidazole membranes containing up to 95 wt% phosphoric acid. Diamino-terminal pre-polymers of different chain lengths are first prepared, followed by addition of a trifunctional carboxylic acid. The crude solutions are cast and subsequently heat treated at up to 230 °C, yielding free-standing membranes of networked polybenzimidazole with high proton conductivity at up to 180 °C and encouraging fuel cell performance

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors, Korea Institute of Science and Technology
Authors: Kirkebæk, A. (Intern), Aili, D. (Intern), Henkensmeier, D. (Ekstern), Jensen, J. O. (Intern), Li, Q. (Intern)
Number of pages: 7
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Macromolecular Materials and Engineering
Volume: 302
Issue number: 12
Article number: 1700347
ISSN (Print): 1438-7492
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 2.71 SJR 0.755 SNIP 0.945
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.01 SJR 0.905 SNIP 0.972
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Giant Electrostriction in highly defective oxides: The next generation of electromechanical materials.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Ceramic Engineering & Science
Authors: Santucci, S. (Intern), Esposito, V. (Intern), Pryds, N. (Intern)
Number of pages: 1
Publication date: 2017

Host publication information
Title of host publication: Book of Abstracts, Sustain 2017
Publisher: Technical University of Denmark (DTU)
Article number: M-20
Main Research Area: Technical/natural sciences
Conference: Sustain 2017, Kgs. Lyngby, Denmark, 06/12/2017 - 06/12/2017
Electronic versions:
SustainAbstracts2017c.compressed_130.pdf
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2017
Giant onsite electronic entropy enhances the performance of ceria for water splitting

Previous studies have shown that a large solid-state entropy of reduction increases the thermodynamic efficiency of metal oxides, such as ceria, for two-step thermochemical water splitting cycles. In this context, the configurational entropy arising from oxygen off-stoichiometry in the oxide, has been the focus of most previous work. Here we report a different source of entropy, the onsite electronic configurational entropy, arising from coupling between orbital and spin angular momenta in lanthanide f orbitals. We find that onsite electronic configurational entropy is sizable in all lanthanides, and reaches a maximum value of \( \approx 4.7 \, k_B \) per oxygen vacancy for Ce\(^{4+}\)/Ce\(^{3+}\) reduction. This unique and large positive entropy source in ceria explains its excellent performance for high-temperature catalytic redox reactions such as water splitting. Our calculations also show that terbium dioxide has a high electronic entropy and thus could also be a potential candidate for solar thermochemical reactions.
Giant tunability of the two-dimensional electron gas at the interface of \( \gamma\text{-Al}_2\text{O}_3/\text{SrTiO}_3 \)

Two-dimensional electron gases (2DEGs) formed at the interface between two oxide insulators provide a rich platform for the next generation of electronic devices. However, their high carrier density makes it rather challenging to control the interface properties under a low electric field through a dielectric solid insulator, i.e. in the configuration of conventional field-effect transistors. To surpass this long-standing limit, we used ionic liquids as the dielectric layer for electrostatic gating of oxide interfaces in an electric double layer transistor (EDLT) configuration. Herein, we reported giant tunability of the physical properties of 2DEGs at the spinel/perovskite interface of \( \gamma\text{-Al}_2\text{O}_3/\text{SrTiO}_3 \) (GAO/STO). By modulating the carrier density thus the band filling with ionic-liquid gating, the system experiences a Lifshitz transition at a critical carrier density of \( 3.0 \times 10^{13} \text{ cm}^{-2} \), where a remarkably strong enhancement of Rashba spin-orbit interaction and an emergence of Kondo effect at low temperatures are observed. Moreover, as the carrier concentration depletes with decreasing gating voltage, the electron mobility is enhanced by more than 6 times in magnitude, leading to the observation of clear quantum oscillations. The great tunability of GAO/STO interface by EDLT gating not only shows promise for design of oxide devices with on-demand properties, but also sheds new light on the electronic structure of 2DEG at the non-isostructural spinel/perovskite interface.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Department of Chemistry, Organic Chemistry, Technical University of Denmark, Nanjing University
Pages: 6878–6885
Publication date: 2017
Main Research Area: Technical/natural sciences
Glass transition of poly (methyl methacrylate) filled with nanosilica and core-shell structured silica

Core-shell (CS) nanocomposite particles with 53.4 wt% cross-linked poly (methyl methacrylate) (PMMA) shell of 11.6 nm in thickness were fabricated via miniemulsion polymerization of methyl methacrylate in the presence of modified nanosilica. The influence of nanosilica and CS nanoparticles on glass transition and segmental dynamics of PMMA in the nanocomposites prepared via solution casting was compared. The remarkable depression (≥10 °C) of glass transition temperature ($T_g$) induced by the incorporation of SiO$_2$ and CS was both observed at low loadings. Here, different mechanisms were responsible for the effect of SiO$_2$ and CS on the segmental acceleration of PMMA matrix. The formation of rigid amorphous fraction (RAF) layer around SiO$_2$ with the thickness of 16.4 nm led to the adjacent molecular packing frustration, while the “lubrication” effect of nonwetting interface between the grafted crosslinked chains and matrix chains resulted in the segmental acceleration and the reduction of dynamic fragility.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors, Zhejiang University
Authors: Song, Y. (Ekstern), Bu, J. (Ekstern), Zuo, M. (Ekstern), Gao, Y. (Ekstern), Zhang, W. (. (Intern), Zheng, Q. (Ekstern)
Pages: 141-149
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Polymer
Volume: 127
ISSN (Print): 0032-3861
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 1.163 SJR 1.097 CiteScore 3.59
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.77 SJR 1.207 SNIP 1.253
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.144 SNIP 1.277 CiteScore 3.72
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.326 SNIP 1.613 CiteScore 3.85
Web of Science (2014): Indexed yes
Guest Editorial

In the 1980s and 1990s, progress in fuel cell and battery research evolved mainly around materials development, empirical approaches, and efforts focusing mostly separately on either the microscale (electrodes and electrolytes) or the macroscale (systems, thermodynamics, and balance-of-plant). Since the 2000s, with the advent of more powerful computing and modeling resources, and the general progress in the field, it has seen a shift to the merging of scales, the possibility of 3D probing and quantification with fuel cell stacks and battery packs becoming the focal point. In parallel, disciplines have merged, too: a holistic and a detailed understanding in the range of underlying phenomena of chemistry, physics, materials science, and mechanical engineering has been combined with the addition of the influence of an electrical field or current. This union is essential to achieve the progress needed for the commercial breakthrough expected from the technologies. It became established that both experimental and modeling aspects deserve simultaneous and an equally weighted consideration, and it is recognized that the correspondences between models and experiments deliver among the most valuable advances to the field, due to the level of confidence and insight they provide.
High definition in-situ electro-optical characterization for Roll to Roll printed electronics

Resume: Printed electronics is emerging as a new, large scale and cost effective technology that will be disruptive in fields such as energy harvesting, consumer electronics and medical sensors. The performance of printed organic electronic devices relies principally on the carrier mobility and molecular packing of the polymer semiconductor material. Unfortunately, the analysis of such materials is generally performed with destructive techniques, which are hard to make compatible with in situ measurements, and pose a great obstacle for the mass production of printed electronics devices. A
rapid, in situ, non-destructive and low-cost testing method is needed. In this study, we demonstrate that nonlinear optical microscopy is a promising technique to achieve this goal. Using ultrashort laser pulses we stimulate two-photon absorption in a roll coated polymer semiconductor and map the resulting two-photon induced photoluminescence (TPPL) and second harmonic response. We anticipate that this non-linear optical method will substantially contribute to the understanding of printed electronic devices and demonstrate it as a promising novel tool for non-destructive and facile testing of materials during printing of the device and at any moment during its lifespan. This will help the production and development of high quality printed technologies where the semiconductor material can be accessed by infrared light, such as solar cells, displays and sensors.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Organic Energy Materials
Authors: Pastorelli, F. (Intern)
Number of pages: 1
Publication date: 2017
Event:
Main Research Area: Technical/natural sciences
Links:

Bibliographical note
SYMPOSIUM L: New materials for organic electronics: from synthesis to processing, characterization and device physics (abstract L. 1.6)
Source: PublicationPreSubmission
Source-ID: 134441444
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2017

Highlights from the FP7 Project on Photovoltaics CHEETAH: More Power with Less Material
CHEETAH is an FP7 integrated research project on photovoltaics funded by the European Commission and was initiated by EERA PV. This project is structured into two type of activities: Coordinative and Support actions (CSA) and Joint Research activities (JRA). The CSA focuses on the creation of a long term collaborative platform by developing tools for knowledge sharing, e-learning platforms for training and education, mobility between researchers, efficient use of infrastructures and promoting best practices and standards. The JRA focuses on developing new concepts and technologies for wafer-based crystalline silicon PV (modules with thin cells < 100 micron), thin-film PV (advanced light management) and organic PV (very low-cost barriers), resulting in reduced cost of environmentally benign/abundant/non-toxic materials and increased module performance. This paper gives a summary of the main achievements of this project for the two categories of activities.

General information
State: Published
Authors: Kroon, J. M. (Ekstern), Roca, F. (Ekstern), Lauermann, I. (Ekstern), Bittkau, K. (Ekstern), Heisz, M. (Ekstern), Van Nieuwenhuysen, K. (Ekstern), Danel, A. (Ekstern), Sommeling, P. (Ekstern), Schmidt, M. (Ekstern), Gevorgyan, S. (Intern)
Pages: 2844-2848
Publication date: 2017

Host publication information
Title of host publication: Proceedings of the 33rd international conference on European Photovoltaic Solar Energy Conference and Exhibition
ISBN (Print): 3936338477
Main Research Area: Technical/natural sciences
DOI:
10.4229/EUPVSEC20172017-7EO.3.5
Publication: Research - peer-review › Article in proceedings – Annual report year: 2018

Highly Conformal Ni Micromesh as a Current Collecting Front Electrode for Reduced Cost Si Solar Cell
Despite relatively high manufacturing cost, crystalline-Si solar cell continues to hold promising future due to its high energy conversion efficiency and long life. As regards cost, one pertinent issue is the top electrode metallization of textured cell surface, which typically involves screen printing of silver paste. The associated disadvantages call for alternative methods that can lower the cost without compromising the solar cell efficiency. In the present work, a highly interconnected one-
dimensional (1D) metal wire network has been employed as front electrode on conventional Si wafers. Here, for the first time, we report an innovative solution based crackle templating method for conformal metal wire network patterning over large textured surfaces. Laser beam induced current mapping showed uniform photocurrent collection by the electrodes without any shadow losses. With electroless deposition of Ni wire network on corrugated solar cell, a short circuit current of 33.28 mA/cm² was obtained in comparison to 20.53 mA/cm² without the network electrode. On comparing the efficiency with the conventional cells with screen printed electrodes, a 20% increment in efficiency has been observed. Importantly, the estimated manufacturing cost is at least two orders lower.

**General information**
State: Published
Authors: Gupta, N. (Ekstern), Rao, K. D. M. (Ekstern), Gupta, R. (Intern), Krebs, F. C. (Intern), Kulkarni, G. U. (Ekstern)
Pages: 8634-8640
Publication date: 2017
Main Research Area: Technical/natural sciences

**Publication information**
Journal: ACS Applied Materials and Interfaces
Volume: 9
Issue number: 10
ISSN (Print): 1944-8244
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 8.15 SJR 2.784 SNIP 1.543
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 7.6 SJR 2.561 SNIP 1.536
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 2.262 SNIP 1.555 CiteScore 7.38
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.125 SNIP 1.636 CiteScore 6.88
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.992 SNIP 1.548 CiteScore 6.05
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.199 SNIP 1.327 CiteScore 4.94
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.046 SNIP 1.404 CiteScore 4.41
ISI indexed (2011): ISI indexed no
Web of Science (2011): Indexed yes
Scopus rating (2010): SJR 1.597 SNIP 0.944
Web of Science (2010): Indexed yes
Web of Science (2009): Indexed yes
Original language: English
Si solar cell, Crackle lithography, Photovoltaics, Solution process, Top contact metallization
DOIs:
10.1021/acsmami.6b12588
Source: FindIt
Source-ID: 2352493759
Publication: Research - peer-review › Journal article – Annual report year: 2017
High performance LaNi$_{1-x}$Co$_x$O$_{3-\delta}$ (x = 0.4 to 0.7) infiltrated oxygen electrodes for reversible solid oxide cells

Oxygen electrodes prepared by infiltration of yttria stabilized zirconia backbone with Ce$_{0.8}$Gd$_{0.2}$O$_{1.95}$ barrier layer and LaNi$_{1-x}$Co$_x$O$_{3-\delta}$ (x = 0.4 to 0.7) catalyst for application in reversible solid oxide cells have been studied. The effect of temperature and Ni:Co ratio on their phase composition, microstructure and electrochemical properties are discussed. It was shown that oxygen electrodes infiltrated with LaNi$_{0.5}$Co$_{0.5}$O$_{3-\delta}$ had the lowest polarization resistance, i.e. 67 mΩ cm$^2$ at 600 °C. The performance of a fuel electrode supported solid oxide cell with infiltrated oxygen electrode in both fuel cell and electrolysis mode was tested. Electrochemical characterization of the solid oxide cell showed that the resistance contribution from these oxygen electrodes to the overall cell resistance is minor i.e. approximately 20 mΩ cm$^2$ at a temperature of 700 °C. The cell was also tested in the steam electrolysis mode at a constant current of −1.0 A cm$^{-2}$ at 800 °C for 240 h. The oxygen electrode showed reasonable degradation rate with the oxygen electrode resistance of 33 mΩ cm$^2$ at 700 °C after 240 h of testing.
High throughput in situ scattering of roll-to-roll coated functional polymer films
The development of conjugated polymers for organic electronics and photovoltaics has relied heavily on advanced X-ray scattering techniques almost since the earliest studies in the field. Almost from the beginning, structural studies focused on how the polymers self-organize in thin films, and the relation between chemical configuration of the polymer, structure and performance. This chapter presents the latest developments where structural analysis is applied as in situ characterization of structure formation during roll-to-roll coating of photoactive layers for solar cells.

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Department of Energy Conversion and Storage, Imaging and Structural Analysis
Authors: Andreasen, J. W. (Intern)
How covalence breaks adsorption-energy scaling relations and solvation restores them

It is known that breaking the scaling relations between the adsorption energies of *O, *OH, and *OOH is paramount in catalyzing more efficiently the reduction of O2 in fuel cells and its evolution in electrolyzers. Taking metalloporphyrins as a case study, we evaluate here the adsorption energies of those adsorbates on the metal centers Cr, Mn, Fe, Co, Ni and Cu, using H, F, OH, NH2, CH3, and BH2 as ring ligands. We show that covalence systematically breaks scaling relations under vacuum by strengthening certain M-OOH bonds. However, covalence modifies adsorbate solvation in solution depending on the degree of covalence of the metal-adsorbate bonds. The two effects have similar magnitudes and opposite signs, such that scaling relations are restored in solution. Thus, solvation is a crucial ingredient that must be taken into account in studies aimed at breaking scaling relations in solution. Our findings suggest that the choice of metal and ligand determines the catalytic activity within the limits imposed by scaling relations, whereas the choice of an appropriate solvent can drive such activity beyond those limits.
Hydrogen Decrepitation Press-Less Process Recycling of NdFeB sintered magnets

A Hydrogen Decrepitation Press-Less Process (HD-PLP) recycling method for recycling of anisotropic NdFeB magnets is demonstrated. The method combines hydrogen decrepitation (HD) disintegration of the initial magnet, powder sieving and the Press-Less Process (PLP), where hydride powder is sintered in a graphite mold. Coercivities up to 534 kA/m were obtained in porous samples based on powder size d < 100 μm. Adding a ball milling step resulted in full density isotropic magnets for d > 100 μm. The coercivity reached Hci = 957 kA/m being 86 % of the original N48M material without addition of rare earth elements.

General information

State: Published
Authors: Xia, M. (Intern), Abrahamsen, A. B. (Intern), Bahl, C. (Intern), Veluri, B. (Ekstern), Søegaard, A. I. (Ekstern), Bøjsøe, P. (Ekstern)
Pages: 55-61
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information

Journal: Journal of Magnetism and Magnetic Materials
Volume: 441
ISSN (Print): 0304-8853
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SJR 0.786 SNIP 1.349 CiteScore 2.97
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.41 SJR 0.699 SNIP 1.181
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.73 SNIP 1.296 CiteScore 2.33
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.815 SNIP 1.423 CiteScore 2.07
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.801 SNIP 1.385 CiteScore 2.03
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
In situ electrical and thermal monitoring of printed electronics by two-photon mapping

Printed electronics is emerging as a new, large scale and cost effective technology that will be disruptive in fields such as energy harvesting, consumer electronics and medical sensors. The performance of printed electronic devices relies principally on the carrier mobility and molecular packing of the polymer semiconductor material. Unfortunately, the analysis of such materials is generally performed with destructive techniques, which are hard to make compatible with in situ measurements, and pose a great obstacle for the mass production of printed electronics devices. A rapid, in situ, non-destructive and low-cost testing method is needed. In this study, we demonstrate that nonlinear optical microscopy is a promising technique to achieve this goal. Using ultrashort laser pulses we stimulate two-photon absorption in a roll coated polymer semiconductor and map the resulting two-photon induced photoluminescence and second harmonic response. We show that, in our experimental conditions, it is possible to relate the total amount of photoluminescence detected to important material properties such as the charge carrier density and the molecular packing of the printed polymer material, all with a spatial resolution of 400 nm. Importantly, this technique can be extended to the real time mapping of the polymer semiconductor film, even during the printing process, in which the high printing speed poses the need for equally high acquisition rates.
Impact of Prosumers and their Clusters on the Energy System

General information
State: Published
Organisations: Department of Civil Engineering, Section for Building Energy, Department of Energy Conversion and Storage, Centre for IT-Intelligent Energy Systems in Cities
Authors: Larma, M. (Intern), Heller, A. (Intern), Pedersen, A. S. (Intern)
Number of pages: 1
Publication date: 2017
Event: Poster session presented at Fourth General CITIES Consortium Meeting, Aarhus, Denmark.
Main Research Area: Technical/natural sciences
Electronic versions: Untitled.pdf
Improved performance of $\text{LaNi}_{0.6}\text{Fe}_{0.4}\text{O}_3$ solid oxide fuel cell cathode by application of a thin interface cathode functional layer

In this work, novel functional layers were prepared by a low temperature spray pyrolysis method on the oxygen side of the solid oxide cells. Thin layers of Ce$0.8$Gd$0.2$O$2$ and LaNi$0.6$Fe$0.4$O$3$ are prepared between the electrolyte and the porous oxygen electrode. Additionally, the influence of the sprayed ceria barrier layer on the zirconia based electrolyte with the new layers is evaluated. Impedance spectroscopy results show improvement in contact between the electrolyte and the porous cathode electrode. Additionally, electrochemical performance of the cathode is improved, as evidenced by a lowered area specific resistance and increased power density obtained from an anode supported cell employing the new layer.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Gdansk University of Technology
Authors: Molin, S. (Intern), Jasinski, P. Z. (Ekstern)
Number of pages: 4
Pages: 252-255
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Materials Letters
Volume: 189
ISSN (Print): 0167-577x
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SJR 0.782 SNIP 0.887 CiteScore 2.68
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.51 SJR 0.754 SNIP 0.939
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.767 SNIP 0.993 CiteScore 2.5
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.877 SNIP 1.28 CiteScore 2.64
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.824 SNIP 1.221 CiteScore 2.41
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.917 SNIP 1.383 CiteScore 2.41
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.014 SNIP 1.546 CiteScore 2.54
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.056 SNIP 1.276
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.038 SNIP 1.268
Improving, characterizing and predicting the lifetime of organic photovoltaics: Topical Review

This review summarizes the recent progress in the stability and lifetime of organic photovoltaics (OPVs). In particular, recently proposed solutions to failure mechanisms in different layers of the device stack are discussed comprising both structural and chemical modifications. Upscaling is additionally discussed from the perspective of stability presenting the challenges associated with device packaging and edge protection. An important part of device stability studies is the characterization, and this review provides a short overview of the most advanced techniques for stability characterization reported recently. Lifetime testing and determination is another challenge in the field of organic solar cells and the final sections of this review discuss the testing protocols as well as the generic marker for device lifetime and the methodology for comparing all the lifetime landmarks in one common diagram. These tools were used to determine the baselines for OPV lifetime tested under different ageing conditions. Finally, the current status of lifetime for organic solar cells is presented and predictions are made for progress in the near future.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Organic Energy Materials
Pages: 1-35
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Volume: 50
Issue number: 10
ISSN (Print): 0022-3727
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 2.38 SJR 0.717 SNIP 1.011
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.07 SJR 1.135 SNIP 1.122
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.886 SNIP 1.25 CiteScore 2.1
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.096 SNIP 1.408 CiteScore 2.53
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.194 SNIP 1.452 CiteScore 2.6
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.279 SNIP 1.414 CiteScore 2.31
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.266 SNIP 1.399 CiteScore 2.36
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.292 SNIP 1.28
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.269 SNIP 1.327
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.427 SNIP 1.549
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.38 SNIP 1.612
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.406 SNIP 1.742
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.216 SNIP 1.455
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.133 SNIP 1.438
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 0.912 SNIP 1.221
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 1.033 SNIP 1.233
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.925 SNIP 1.212
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 0.842 SNIP 1.125
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 0.89 SNIP 1.264

Original language: English

Organic photovoltaics, Lifetime, Stability, Degradation, Lifetime testing, Advanced characterization

Electronic versions:
Review_on_Lifetime_of_OPVs_V2.pdf

DOIs:
10.1088/1361-6463/50/10/103001
Source: FindIt
Source-ID: 2352328200

Publication: Research - peer-review › Journal article – Annual report year: 2017
Indoor measurement of angle resolved light absorption by antireflective glass in solar panels

In this work, we present measurements of angle resolved light absorption of antireflective (AR) glass of PV samples, performed indoors using a collimated high radiance broadband light source. This indoor method proved to be viable and offered a significant simplification compared to outdoor measurements with trackers. The experimental results showed optical responses that are stable and suitable for indoor characterization of solar cells. We find the characteristic optical response of six different antireflective glasses, and based on such measurements, we perform PVsyst simulations and present the monthly DC energy production estimates across four distinct latitudinal locations with six different glass types. The results indicated that the AR glasses present different optical effects at the angles intervals between 0 – 45° and 60 – 90° and that the Diffuse AR glass can improve monthly yields by as much as 2% relatively to a bare cell.

General information
State: Published
Organisations: Department of Photonics Engineering, Diode Lasers and LED Systems, Photovoltaic Materials and Systems, Organic Energy Materials, Department of Micro- and Nanotechnology, Silicon Microtechnology, Experimental Surface and Nanomaterials Physics
Number of pages: 4
Publication date: 2017

Host publication information
Title of host publication: Proceedings of the 33rd European Photovoltaic Solar Energy Conference and Exhibition
Main Research Area: Technical/natural sciences
Antireflective glass, Angle of Incidence, Incidence Angle Modifier, Simulation
Electronic versions:
Poster

Indoor Measurement of Angle Resolved Light Absorption by Black Silicon

Angle resolved optical spectroscopy of photovoltaic (PV) samples gives crucial information on PV panels under realistic working conditions. Here, we introduce measurements of angle resolved light absorption by PV cells, performed indoors using a collimated high radiance broadband light source. Our indoor method offers a significant simplification as compared to measurements by solar trackers. As a proof-of-concept demonstration, we show characterization of black silicon solar cells. The experimental results showed stable and reliable optical responses that makes our setup suitable for indoor, angle resolved characterization of solar cells.

General information
State: Published
Organisations: Department of Photonics Engineering, Diode Lasers and LED Systems, Department of Micro- and Nanotechnology, Silicon Microtechnology, Experimental Surface and Nanomaterials Physics, Photovoltaic Materials and Systems, Organic Energy Materials
Number of pages: 3
Publication date: 2017

Host publication information
Title of host publication: Proceedings of the international 2017 IEEE Photovoltaic Specialists Conference
Publisher: IEEE
Main Research Area: Technical/natural sciences
Electronic versions:
Poster

Indoor Measurement of Angle Resolved Absorption of Black Silicon CommentsAddressed BI_Mek_PP_Final_1_.pdf
Source: PublicationPreSubmission
Source-ID: 139805541
Publication: Research - peer-review › Article in proceedings – Annual report year: 2017
Infiltrated La$_{0.4}$Sr$_{0.4}$Fe$_{0.03}$Ni$_{0.03}$Ti$_{0.94}$O$_{3}$ based anodes for all ceramic and metal supported solid oxide fuel cells

For improved robustness, durability and to avoid severe processing challenges alternatives to the Ni:YSZ composite electrode is highly desirable. The Ni:YSZ composite electrode is conventionally used for solid oxide fuel cell and solid oxide electrolysis cell. In the present study we report on high performing nanostructured Ni:CGO electrocatalyst coated A site deficient Lanthanum doped Strontium Titanate (La0.4Sr0.4Fe0.03Ni0.03Ti0.94O3) based anodes. The anodes were incorporated into the co-sintered DTU metal supported solid oxide fuel cell design and large sized 12 cm × 12 cm cells were fabricated. The titanate material showed good processing characteristics and surface wetting properties towards the Ni:CGO electrocatalyst coating. The cell performances were evaluated on single cell level (active area 16 cm$^2$) and a power density at 0.7 V and 700 °C of 0.650 Wcm$^{-2}$ with a fuel utilization of 31% was achieved. Taking the temperature into account the performances of the studied anodes are among the best reported for redox stable and corrosion resistant alternatives to the conventional Ni:YSZ composite solid oxide cell electrode.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry, Mixed Conductors, Ceramic Engineering & Science, Imaging and Structural Analysis, University of St Andrews
Authors: Nielsen, J. (Intern), Persson, Å. H. (Intern), Sudireddy, B. R. (Intern), Irvine, J. T. (Ekstern), Thydén, K. T. S. (Intern)
Pages: 99-106
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Power Sources
Volume: 372
ISSN (Print): 0378-7753
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 7 SJR 2.202 SNIP 1.536
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 6.22 SJR 1.944 SNIP 1.5
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.9 SNIP 1.667 CiteScore 6.34
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.964 SNIP 2.042 CiteScore 6.3
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.975 SNIP 2.137 CiteScore 5.63
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.282 SNIP 2.006 CiteScore 5.04
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.227 SNIP 2.172 CiteScore 5.13
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 2.294 SNIP 1.972
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Influence of carbon monoxide on the cathode in high-temperature polymer electrolyte membrane fuel cells

This paper describes the results of adding small amounts of CO gas to the cathode side in a HT-PEM fuel cell with a polybenzimidazole (PBI) membrane running on either oxygen or air. Experimental conditions: Temperature ranges 120–160 °C, constant current either 200 mA/cm² or 800 mA/cm² and CO ranges 0.1–1.3%. In this case it was found that small amounts of CO under special conditions have a beneficial effect on the potential of the fuel cells, whereas larger amounts can bring the potential down to almost zero. An interesting phenomenon is that after the flow of CO is switched off a temporary improvement of the potential is seen before the situation goes back to normal. A good explanation for this is a competition between CO, O₂ and H₃PO₄ at the three phase boundaries, also that a steady state exist in which CO constantly is oxidized to CO₂.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors
Authors: Søndergaard, S. (Intern), Cleemann, L. N. (Intern), Jensen, J. O. (Intern), Bjerrum, N. J. (Intern)
Pages: 3309-3315
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Volume: 42
Issue number: 5
ISSN (Print): 0360-3199
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 4.1 SJR 1.116 SNIP 1.267
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.74 SJR 1.145 SNIP 1.315
The aim of this work is to assess the influence of a magnetic sample on the applied magnetic field inside the air gap of a magnetic circuit. Different magnetic sources including an electromagnet, a permanent magnet in a soft ferromagnetic toroidal yoke, as well as 2D and 3D Halbach cylinders are considered, using a numerical model. Gadolinium is chosen as magnetic material for the sample, due to its strong magnetocaloric properties and its wide use in magnetic refrigeration prototypes. We find that using uniform theoretical demagnetizing factors for cylinders or spheres results in a deviation of less than 2% in the calculation of internal magnetic fields at temperatures above the Curie point of gadolinium. Below the Curie point, a stronger magnetization of the cylinders and spheres leads to a larger deviation which can reach 8% when
using uniform demagnetizing factors for internal magnetic field calculations.
Influence of Substrate-Film Reactions on YBCO Grown by Fluorine-Free MOD Route

Recently, fluorine-free metal organic deposition routes (FF-MOD) for growth of YBCO superconducting films have attracted increased attentions. In this paper, a comparison study was performed on the YBCO-Ag superconducting thin films deposited on two types substrates, LaAlO3 and CSD-Ce0.9La0.1O2-y (CLO)/YSZ, respectively. Although conventional TFA-MOD derived YBCO films exhibit high performance on both substrates, the results vary when using the FF-MOD precursor. SEM and XRD results reveal that c-axis and a/b-axis orientations coexist in the YBCO-Ag films grown on the CLO/YSZ substrate deposited by the FF-MOD route, while the BaCeO3 by-product is a dominating phase in the fully reacted film. Based on the structural analysis of the partially converted films, we found that interfacial reactions between the film and the CLO cap layer play an essential role on the epitaxial growth of YBCO-Ag films from the FF-MOD solution. Because of the different chemical reaction path compared to conventional TFA-MOD routes, it seems that the polycrystalline BaCeO3 formation takes place prior to the YBCO-Ag epitaxial growth associated with the melting process, which results in structural deterioration at high growth temperatures and, therefore, no superconductivity. This study indicates the necessity of further reducing the nucleation temperature of YBCO films processed by FF-MOD routes.

General information

State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Shanghai Jiao Tong University
Authors: Zhao, Y. (Ekstern), Tang, X. (Intern), Wu, W. (Ekstern), Grivel, J. (Intern)
Number of pages: 4
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information

Journal: IEEE Transactions on Applied Superconductivity
Volume: 27
Issue number: 4
ISSN (Print): 1051-8223
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 1.45 SJR 0.408 SNIP 0.962
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.42 SJR 0.398 SNIP 1.145
Web of Science (2016): Indexed yes
Fluorine-free solution, YBCO films, All-chemical-solution route, Interface reaction

Influence of yttria surface modification on high temperature corrosion of porous Ni22Cr alloy

Protective coatings for porous alloys for high temperature use are relatively new materials. Their main drawback is high temperature corrosion. In this work protective coatings based the on Y-precursor infiltrated into the sintered Ni22Cr alloys are studied at 700°C. Effects of the amount of the protective phase on the resulting corrosion properties are evaluated in air and humidified hydrogen. Weight gain of the samples, their open porosities and microstructures are analyzed and compared. Results show, that by the addition of even a minor amount of the Y-precursor corrosion rates can be decreased by a factor of 50.

General information
State: Published
Initiative Towards Non-Precious Metal Polymer Fuel Cells (NonPrecious)

General information
State: Published
Authors: Jensen, J. O. (Intern), Shypunov, I. (Intern), Cleemann, L. N. (Intern), Li, Q. (Intern), Hansen, H. A. (Intern), Vegge, T. (Intern), Holst-Olesen, K. (Forskerdatabase), Zana, A. (Ekstern), Arenz, M. (Ekstern), Hjuler, H. A. (Ekstern), Steenberg, T. (Ekstern), Juul Larsen, M. (Ekstern), Sun, S. (Ekstern), Dodelet, J. (Ekstern), Shen, P. (Ekstern)
Number of pages: 1
Publication date: 2017
Main Research Area: Technical/natural sciences
Electronic versions:
NonPrecious_Jens_Oluf_Jensen
Source: PublicationPreSubmission
Source-ID: 141975597
Publication: Research › Conference abstract for conference – Annual report year: 2017
In-line, roll-to-roll morphology analysis of organic solar cell active layers

We present the first comparative in situ small and wide angle X-ray scattering study of two polymers that are relevant for organic photovoltaics, during coating on a flexible substrate. From the obtained measurements we identified several differences between the drying of the two polymers. The polymer optimized for roll-to-roll coating attained its final morphological packing nearly instantly after deposition, and had the shortest drying profile. We therefore conclude that fast-drying polymers which are influenced less by drying temperature or substrate inhomogeneities are better suited for roll-to-roll coating, and that fundamentally, the kinetics of drying dominate the process in the case of roll-to-roll slot-die coating.

General information
State: Published
Pages: 2411-2419
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Energy & Environmental Science
Volume: November
Issue number: 11
ISSN (Print): 1754-5692
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): SNIP 4.819 SJR 14.59 CiteScore 30.87
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 26.39 SJR 12.283 SNIP 4.325
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 7.769 SNIP 4.001 CiteScore 19.28
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 6.019 SNIP 2.996 CiteScore 14.81
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 5.868 SNIP 2.599 CiteScore 11.84
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 3.737 SNIP 2.505 CiteScore 9.96
ISI indexed (2011): ISI indexed no
Web of Science (2011): Indexed yes
Scopus rating (2010): SJR 3.87 SNIP 2.42
Web of Science (2010): Indexed yes
Scopus rating (2009): SJR 2.111 SNIP 1.15
Original language: English
DOIs:
10.1039/C7EE01900A
**In operando Raman spectroscopy for investigation of solid oxide electrolysis cells**

**Summary.** How can in operando Raman spectroscopy increase our understanding of degradation and activation processes in solid oxide electrolysis cells? Recent experimental results are reported, including experiments showing remarkable polarisation induced compositional changes in infiltrated perovskite electrodes.

**General information**
State: Published
Organisations: Department of Energy Conversion and Storage, Montana State University
Authors: Traulsen, M. L. (Intern), Walker, R. A. (Ekstern), Holtappels, P. (Intern)
Number of pages: 1
Pages: 167
Publication date: 2017

**Host publication information**
Title of host publication: 1st International Conference on Electrolysis - Book of abstracts
Main Research Area: Technical/natural sciences
Conference: Copenhagen, Denmark, 12/06/2017 - 12/06/2017
Electronic versions:
ICE2017_Traulsen_Marie_abstract.pdf
Links:
http://www.ice2017.net/Conference
Source: PublicationPreSubmission
Source-ID: 138261362
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2017

**In Operando Raman spectroscopy for investigation of solid oxide electrolysis cells**

**General information**
State: Published
Organisations: Department of Energy Conversion and Storage, Montana State University
Authors: Traulsen, M. L. (Intern), Walker, R. A. (Ekstern), Holtappels, P. (Intern)
Number of pages: 1
Publication date: 2017
Event: Poster session presented at International Conference on Electrolysis, Copenhagen, Denmark.
Main Research Area: Technical/natural sciences
Electronic versions:
2017_ICE_conference_poster_matr_.pdf
Publication: Research › Poster – Annual report year: 2017

**In operando studies of an yttria stabilized zirconia electrolyte supported symmetric solid oxide cell by Dark field X-ray Microscopy at ID06**

**General information**
State: Published
Organisations: Department of Energy Conversion and Storage, Imaging and Structural Analysis, Neutrons and X-rays for Materials Physics, Department of Physics, ESRF Beamline
Authors: Sierra, J. X. (Intern), Jørgensen, P. S. (Intern), Poulsen, H. F. (Intern), Detlefs, C. (Ekstern), Cook, P. (Ekstern), Simon, H. (Intern), Bowen, J. R. (Intern)
Number of pages: 1
Publication date: 2017
Main Research Area: Technical/natural sciences
Electronic versions:
Poster_Microsymposia_JXST_.pdf
Source: PublicationPreSubmission
Source-ID: 143955620
Publication: Research › Poster – Annual report year: 2018

**In operando studies of an yttria stabilized zirconia electrolyte supported symmetric solid oxide cell by Dark field X-ray Microscopy at ID06**
**General information**  
**State:** Published  
**Organisations:** Department of Energy Conversion and Storage, Imaging and Structural Analysis, Neutrons and X-rays for Materials Physics, Department of Physics, ESRF Beamline  
**Authors:** Sierra, J. X. (Intern), Jørgensen, P. S. (Intern), Poulsen, H. F. (Intern), Detlefs, C. (Ekstern), Cook, P. (Ekstern), Simons, H. (Intern), Bowen, J. R. (Intern)  
**Number of pages:** 1  
**Publication date:** 2017  
**Event:** Abstract from ESRF User Meeting 2017, Grenoble, France.  
**Main Research Area:** Technical/natural sciences  
**Electronic versions:**  
**Abstract_JXST.pdf**  
**Publication: Research › Conference abstract for conference – Annual report year: 2018**

**In operando studies of ScYSZ electrolyte supported symmetric solid oxide cell by X-ray Diffraction at ESRF, ID06 Beamline**

Solid Oxide Cells are becoming a promising solution for sustainable and renewable power generation. Scandium doped Yttria Stabilized Zirconia is considered one of the best materials used as electrolyte because of its high ionic conductivity and great mechanical and chemical stability under operating conditions. Oxygen bubble formation at grain boundaries of ScYSZ near the anode/electrolyte interface has been observed as a degradation process when running in electrolysis mode at 800 - 900 oC for 24 - 72 hours at high current densities. X-ray diffraction can provide information about structural evolution at different depths of the cell during operation.

---

**General information**  
**State:** Published  
**Organisations:** Department of Energy Conversion and Storage, Imaging and Structural Analysis, Neutrons and X-rays for Materials Physics, Department of Physics, ESRF Beamline  
**Number of pages:** 1  
**Publication date:** 2017  
**Event:** Poster session presented at 3rd International Conference on Tomography of 3D Materials and Structures, Lund, Sweden.  
**Main Research Area:** Technical/natural sciences  
**Electronic versions:**  
**Poster_ICTMS_2017_JXST_.pdf**  
**Source:** PublicationPreSubmission  
**Source-ID:** 143956251  
**Publication: Research › Poster – Annual report year: 2018**

**In operando study of high-performance thermoelectric materials for power generation: a case study of β-Zn₄Sb₃**

To bring current thermoelectric (TE) materials achievement into a device for power generation, a full understanding of their dynamic behavior under operating conditions is needed. Here, an in operando study is conducted on the high-performance TE material β-Zn₄Sb₃ under large temperature gradient and thermal cycling via a new approach using in situ transmission electron microscopy combined with characterization of the TE properties. It is found that after 30 thermal cycles in a low-pressure helium atmosphere the TE performance of β-Zn₄Sb₃ is maintained with the figure of merit, zT, value of 1.4 at 718 K. Under a temperature gradient of 380 K (T_{hot} = 673 K and T_{cold} = 293 K) operating for only 30 h, zinc whiskers gradually precipitate on the cold side of the β-Zn₄Sb₃ leg. The dynamical evolution of Zn in the matrix of β-Zn₄Sb₃ is found to be the source that leads to a high zT value by lowering of the thermal conductivity and electrical resistivity, but it is also the failure mechanism for the leg under these conditions. The in operando study brings deep insight into the dynamic behavior of nanostructured TE materials for tailoring future TE materials and devices with higher efficiency and longer durability.

---

**General information**  
**State:** Published  
**Organisations:** Department of Energy Conversion and Storage, Mixed Conductors, Electrofunctional materials, Ceramic Engineering & Science, TEGnology ApS, Aarhus University  
**Authors:** Le, T. H. (Intern), Ngo, D. (Intern), Han, L. (Intern), Iversen, B. B. (Ekstern), Yin, H. (Ekstern), Pryds, N. (Intern), Van Nong, N. (Intern)  
**Number of pages:** 17  
**Publication date:** 2017  
**Main Research Area:** Technical/natural sciences
Inside or Outside? Linking Outdoor and Indoor Lifetime Tests of ITO-Free Organic Photovoltaic Devices for Greenhouse Applications

We present results from an installation of fully roll-to-roll printed and coated polymer solar cell modules in a greenhouse environment over the course of roughly 2 years (650 days). We explored two different device architectures based on either fully carbon-based electrodes or silver nanowire (AgNW)-based electrodes and two different barrier materials. We followed the ISOS protocols while studying the devices in three different greenhouse conditions in the Netherlands and compared to reference devices mounted outdoors in Denmark tested according to ISOS-O-1 and ISOS-O-2. We studied each condition and type in multiples to obtain acceptable statistics and found that the AgNW-based devices performed best in terms of stability.

General information
State: Published
Authors: Benatto, G. A. D. R. (Intern), Corazza, M. (Intern), Roth, B. (Intern), Schütte, F. (Ekstern), Rengenstein, M. (Ekstern), Gevorgyan, S. (Intern), Krebs, F. C. (Intern)
Pages: 338-344
Publication date: 2017
Main Research Area: Technical/natural sciences

In-situ formed Ce$_{0.8}$Gd$_{0.2}$O$_{1.9}$ barrier layers on yttria stabilized zirconia backbones by infiltration - A promising path to high performing oxygen electrodes of solid oxide cell
Oxygen electrodes for solid oxide cells were prepared by a consecutive infiltration of a gadolinium doped ceria (Ce$_{0.8}$Gd$_{0.2}$O$_{1.9}$, CGO) barrier layer and a lanthanum cobalt nickelate (La$_{0.95}$Co$_{0.4}$Ni$_{0.6}$O$_3$, LCN) electro catalyst layer into a porous yttrium doped zirconia (YSZ) backbone. The influences of the following parameters on the microstructure of the formed CGO barrier layer and on the electrochemical performance of the cells were studied: i) surfactants and wetting agents, ii) ceria/gadolinia coverage, iii) calcination profiles and iv) exposure temperature during testing. The infiltration process of the CGO barrier layer was optimized and a slow, pH controlled decomposition of urea containing precursor solutions was found to be most effective. For these cells a decrease of 84% in the polarization resistance ($R_p$) was achieved compared to cells without a barrier layer. Furthermore, a better initial performance and only a small increase of the cell-resistance with increasing exposure temperatures during testing were obtained. A complete and homogenous covering of the YSZ backbone with Ce$_{0.8}$Gd$_{0.2}$O$_{1.9}$ was found to be necessary to maintain high performance also at higher exposure temperatures (> $800^\circ$C).

**General information**
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors
Pages: 51-59
Publication date: 2017
Main Research Area: Technical/natural sciences

**Publication information**
Journal: Solid State Ionics
Volume: 304
ISSN (Print): 0167-2738
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 2.64 SJR 0.856 SNIP 0.952
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.41 SJR 0.75 SNIP 0.909
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.802 SNIP 1.016 CiteScore 2.5
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.837 SNIP 1.282 CiteScore 2.62
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.903 SNIP 1.269 CiteScore 2.35
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.051 SNIP 1.253 CiteScore 2.31
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.376 SNIP 1.615 CiteScore 2.96
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.46 SNIP 1.498
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.508 SNIP 1.483
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
In Situ Formed Phosphoric Acid/Phosphosilicate Nanoclusters in the Exceptional Enhancement of Durability of Polybenzimidazole Membrane Fuel Cells at Elevated High Temperatures

Most recently, we developed a phosphotungstic acid impregnated mesoporous silica (PWA-meso-silica) and phosphoric acid doped polybenzimidazole (PA/PBI) composite membrane for use in high temperature fuel cells and achieved exceptional durability under a constant current load of 200 mA cm$^{-2}$ at 200°C for over 2700 h. In this work, the fundamental role of PWA-meso-silica in enhancing the stability of the PA/PBI membrane has been investigated. The microstructure, the PA uptake, swelling ratio, mechanical property and conductivity of PA/PBI/PWA-meso-silica composite membranes depend on the loading of PWA-meso-silica. The results indicate that the optimum limit of PWA-meso-silica loading in the PA/PBI membranes is 15 wt%. Detailed analysis indicates that the mesoporous structure of the PWA-meso-silica framework disintegrates, forming phosphosilicate phases within the PBI polymeric matrix during fuel cell operation at 200°C. The in situ formed phosphosilicates can immobilize a significant amount of PA, forming PA/phosphosilicate nanoclusters that possess high proton conductivity (e.g., 7.2 × 10$^{-2}$ S cm$^{-1}$ at 250°C) and stability and substantially inhibits acid leaching out of the membrane. The substantially reduced acid leaching also alleviates the excess acid in the catalyst layer, reducing the detrimental effect of excess acid on the agglomeration of Pt catalysts especially in the cathode catalyst layer. These phenomena are responsible for the exceptional stability in proton conductivity as well as the significantly reduced agglomeration of Pt nanoparticles in the anode and cathode catalyst layers of PA/PBI/PWA-meso-silica composite membrane fuel cells.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors, Beihang University, University of the Sunshine Coast, Curtin University
Authors: Zhang, J. (Ekstern), Aili, D. (Intern), Bradley, J. (Ekstern), Kuang, H. (Ekstern), Pan, C. (Intern), De Marco, R. (Ekstern), Li, Q. (Intern), Jiang, S. P. (Ekstern)
Pages: F1615-F1625
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of the Electrochemical Society
Volume: 164
Issue number: 14
ISSN (Print): 0013-4651
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 3.48 SJR 1.267 SNIP 1.009
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.97 SJR 1.222 SNIP 0.963
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.115 SNIP 1.066 CiteScore 3.17
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.213 SNIP 1.25 CiteScore 3.36
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.169 SNIP 1.309 CiteScore 2.92
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.329 SNIP 1.281 CiteScore 2.61
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.331 SNIP 1.335 CiteScore 2.74
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.418 SNIP 1.304
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.442 SNIP 1.27
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.595 SNIP 1.41
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.569 SNIP 1.322
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.608 SNIP 1.535
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.523 SNIP 1.481
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.712 SNIP 1.7
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.971 SNIP 1.677
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 2.036 SNIP 1.618
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 1.663 SNIP 1.729
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 1.632 SNIP 1.7
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 1.6 SNIP 1.846
Original language: Undefined/Unknown
In situ TEM analysis of a symmetric solid oxide cell in oxygen and vacuum–cation diffusion observations

In order to establish the use of solid oxide fuel/electrolysis cells (SOFC/SOEC) in the energy market, a deeper understanding of degradation effects during operation is necessary. This study applies in situ transmission electron microscopy (TEM) of a symmetric model cell composed by two oxygen electrodes of La$_{0.6}$Sr$_{0.4}$CoO$_{3-δ}$ (LSC) and an electrolyte, ZrO$_2$: 8% mol Y$_2$O$_3$ (8YSZ), deposited on 1% Nb doped SrTiO$_{3-δ}$ (STN) single crystal substrate by pulsed laser deposition. The results showed a high cation mobility of the electrodes when exposed to 900 ºC. Cobalt is found to agglomerate at the interface between LSC and STN. Strontium depletion is observed in both electrodes. Finally, a faster grain growth occurs in LSC for the cell exposed to oxygen in comparison with the cell in vacuum.
In situ TEM study of the coarsening of carbon black supported Pt nanoparticles in hydrogen

The control of sizes and shapes of nanostructures is of tremendous importance for the catalytic activity in electrochemistry and in catalysis more generally. However, due to relatively large surface free energies, nanostructures often sinter to form coarser and more stable structures that may not have the intended physicochemical properties.

Pt is known to be a very active catalyst in several chemical reactions and for example as carbon supported nanoparticles in fuel cells.

The presentation focusses on coarsening mechanisms of Pt nanoparticles supported on carbon black during exposure to hydrogen. By means of in situ transmission electron microscopy (TEM), Pt nanoparticle coarsening was monitored in 6 mbar 20 % H2/Ar while ramping up the temperature to ca. 900 °C. Time-resolved TEM images directly reveal that separated ca. 3 nm sized Pt nanoparticles in the pure hydrogen environment are stable during constant temperature ramping by 10°C/min up to ca. 800 °C. The coarsening above this temperature is fully dominated by the particle migration and coalescence mechanism. This is contrary to supported Pt nanoparticles in oxygen, where the coarsening is fully dominated by Ostwald ripening. For agglomerated Pt nanoparticles, coalescence events were observed already at ca. 200 °C. The temperature-dependency of particle sizes and the observed migration distances are consistent with simple early models for the migration and coalescence.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Imaging and Structural Analysis, Proton conductors, Huaihai Institution of Technology
Authors: Simonsen, S. B. (Intern), Wang, Y. (Ekstern), Jensen, J. O. (Intern), Zhang, W. (. (Intern)
Number of pages: 1
Publication date: 2017
Conference: 232nd ECS meeting, National Harbor, Washington, DC, United States, 01/10/2017 - 01/10/2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Electrochemical Society. Meeting Abstracts (Online)
Volume: MA2017-02
Article number: 1433
ISSN (Print): 2151-2043
Original language: English
Electronic versions:
2017_Simonsen_ECS_232th_meeting.pdf
Links:
http://ma.ecsd.org/content/MA2017-02/1433.abstract?sid=7d22f381-06cc-4cd6-ab50-980f863bd550
Publication: Research - peer-review › Conference abstract in journal – Annual report year: 2017

In Situ Transmission Electron Microscopy in Materials Science - Possibilities and Prospects

General information
State: Published
Organisations: Center for Electron Nanoscopy, Department of Energy Conversion and Storage, Imaging and Structural Analysis
Authors: Wagner, J. B. (Intern), Zhang, L. (Intern), Gualandris, F. (Intern), Simonsen, S. B. (Intern), Kuhn, L. T. (Intern), Beleggia, M. (Intern), Hansen, T. W. (Intern)
Number of pages: 3
Publication date: 2017
Main Research Area: Technical/natural sciences
Electronic versions:
Untitled.pdf
Intrinsic Conductivity in Magnesium-Oxygen Battery Discharge Products: MgO and MgO2

Nonaqueous magnesium-oxygen (or “Mg-air”) batteries are attractive next generation energy storage devices due to their high theoretical energy densities, projected low cost, and potential for rechargeability. Prior experiments identified magnesium oxide, MgO, and magnesium peroxide, MgO2, as the primary discharge products in a Mg/O2 cell. Charge transport within these nominally insulating compounds is expected to limit battery performance; nevertheless, these transport mechanisms either are incompletely understood (in MgO2) or remain a matter of debate (in MgO). The present study characterizes the equilibrium conductivity associated with intrinsic (point) defects within both compounds using first-principles calculations. For MgO, negative Mg vacancies and hole polarons—the latter localized on oxygen anions—were identified as the dominant charge carriers. However, the large formation energies associated with these carriers suggest low equilibrium concentrations. A large asymmetry in the carrier mobility is predicted: hole polarons are highly mobile at room temperature, while Mg vacancies are essentially immobile. Accounting for nonequilibrium effects such as frozen-in defects, the calculated conductivity data for MgO is shown to be in remarkable agreement with the three “Arrhenius branches” observed in experiments, thus clarifying the long-debated transport mechanisms within these regimes. In the case of MgO2, electronic charge carriers alone—electron and hole polarons—are the most prevalent. Similar to MgO, the equilibrium concentration of carriers in MgO2 is low, and moderate-to-poor mobility further limits conductivity. If equilibrium behavior is realized, then we conclude that (i) sluggish charge transport in MgO or MgO2 will limit battery performance when these compounds cover the cathode support and (ii) what little conductivity exists in these phases is primarily electronic in nature (i.e., polaron hopping). Artificially increasing the carrier concentration via monovalent substitutions is suggested as a strategy for overcoming transport limitations.
Investigating phase behavior and structural changes in NiO/Ni-YSZ composite with monochromatic in-situ 2D and static 3D neutron imaging

In this work, we report neutron imaging studies of redox cycling of NiO/Ni-8YSZ (nickel/nickel oxide – yttria stabilized zirconia) composite used for electrodes in solid oxide electrochemical cells for efficient energy conversion (power-to-gas and vice versa) purposes (i.e. for anodes in solid oxide fuel cells, and for cathodes in solid oxide electrolysis cells). Results of in-situ 2D and ex-situ 3D measurements are presented. In-situ observation of phase transition between NiO and Ni were performed at the test Beamline for neutron Optics and other Applications (BOA) at the continuous neutron source SINQ of Paul Scherrer Institut (PSI, Switzerland) by means of monochromatic neutron imaging, and post mortem monochromatic neutron tomography was performed at Helmholtz Zentrum Berlin (HZB) at the BER II reactor using the CONRAD-2 imaging instrument. Combining both time resolved radiography and post mortem tomography provides complementary information about the reduction/oxidation degree and e.g. crack evolution in the investigated system and it is therefore possible to acquire information about the rate of chemical reactions and spatial evolution of phases and morphological features.

General information
State: Accepted/In press
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Imaging and Structural Analysis, University of Bayreuth, Paul Scherrer Institut, Helmholtz–Zentrum Berlin für Materialien und Energie, Xnovo Technology ApS
Authors: Makowska, M. G. (Ekstern), Strobl, M. (Ekstern), Kardjilov, N. (Ekstern), Frandsen, H. L. (Intern), Manke, I. (Ekstern), Morgano, M. (Ekstern), Lacatusu, M. (Intern), De Angelis, S. (Intern), Lauridsen, E. M. (Ekstern), Kuhn, L. T. (Intern)
Number of pages: 5
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Physica B: Condensed Matter
ISSN (Print): 0921-4526
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 1.45 SJR 0.417 SNIP 0.791
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.39 SJR 0.446 SNIP 0.828
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.475 SNIP 0.809 CiteScore 1.41
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.549 SNIP 0.931 CiteScore 1.45
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.557 SNIP 0.99 CiteScore 1.41
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.589 SNIP 0.887 CiteScore 1.21
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.595 SNIP 0.806 CiteScore 1.13
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Investigation of a Spinel-forming Cu-Mn Foam as an Oxygen Electrode Contact Material in a Solid Oxide Cell Single Repeating Unit

A critical issue in state-of-the-art solid oxide cell stacks is the contacting of the oxygen electrode. The commonly used ceramic contact layers are applied in a green state and cannot be sintered properly, due to compliance limitations arising from other stack components like sealing glasses and steels. The consequence is a low layer and interface strength. A metallic copper manganese foam, which is oxidized under operation conditions into a conductive $\text{Cu}_{1+x}\text{Mn}_{2-x}\text{O}_4$ spinel, is presented in this work as a viable contact solution. The foam has been electrochemically tested in a single repeating unit setup for 350 hours of constant operation, followed by dynamic conditions with thermal cycles. After operation, a microstructural analysis using scanning electron microscopy, energy dispersive X-ray spectroscopy and X-ray diffraction was carried out. It was confirmed that after oxidation/operation the manganese solely formed a CuMn-spinel phase, mixed with a CuO phase. A separate Mn-oxide phase was not found. The conductivity and contacting of the foam was sufficient for > 350 h of SOFC operation. With an initial serial resistance comparable to single cell tests using gold foil as contact material and moderate degradation rates, the CuMn foam presented itself as an interesting cathode contact solution.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Electrofunctional materials, Applied Electrochemistry
Authors: Zielke, P. (Intern), Wulff, A. C. (Intern), Sun, X. (Intern), Jensen, S. H. (Intern), Frandsen, H. L. (Intern), Norby, P. (Intern), Hagen, A. (Intern)
Pages: 730-734
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Fuel Cells
Volume: 17
Issue number: 5
ISSN (Print): 1615-6846
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
Investigation of Cu₂ZnSnS₄ nanoparticles for thin-film solar cell applications

We study the effect of the annealing atmosphere on grain growth of ligand-free and ligand-coated Cu₂ZnSnS₄ (CZTS) nanoparticle-based thin films by thermal analysis. We use thermogravimetric analysis (TGA) coupled with mass spectrometry (MS) to simultaneously monitor mass changes and evolved gases of both nanoparticle powders and inks. The investigation focuses on annealing in air, nitrogen and forming gas (5% H₂ in Ar), i.e., oxidizing, inert, and reducing atmospheres. We find that the oleylamine capping ligands thermally decompose into smaller organic fragments starting...
below its boiling point, with a slightly higher decomposition rate in reducing atmosphere. With nanoparticle inks, very modest grain growth is observed, with no differences between the atmospheres. Conversely, with nanoparticle powders, micron-sized grains appear all over for the ligand-free sample and some micron-sized grains are seen with inert atmosphere for the ligand-coated powder. The starting material is thus very important for grain growth.

**General information**

State: Published
Organisations: Department of Photonics Engineering, Optical Microsensors and Micromaterials, Department of Energy Conversion and Storage, Mixed Conductors, Department of Micro- and Nanotechnology, Silicon Microtechnology, Experimental Surface and Nanomaterials Physics, Nanyang Technological University
Authors: Engberg, S. L. J. (Intern), Agersted, K. (Ekstern), Crovetto, A. (Intern), Hansen, O. (Intern), Lam, Y. M. (Ekstern), Schou, J. (Intern)
Number of pages: 7
Pages: 163-169
Publication date: 2017
Main Research Area: Technical/natural sciences

**Publication information**

Journal: Thin Solid Films
Volume: 628
ISSN (Print): 0040-6090
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 1.91 SJR 0.617 SNIP 0.864
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.83 SJR 0.639 SNIP 0.881
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.68 SNIP 0.923 CiteScore 1.84
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.725 SNIP 1.075 CiteScore 1.94
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.814 SNIP 1.195 CiteScore 2
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.897 SNIP 1.153 CiteScore 1.86
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 0.995 SNIP 1.323 CiteScore 2.13
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.132 SNIP 1.224
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.127 SNIP 1.213
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.182 SNIP 1.275
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.146 SNIP 1.192
Web of Science (2007): Indexed yes
(Invited) Oxygen Exchange Kinetics on Technological Versus Model Type Electrodes

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors
Authors: Hendriksen, P. V. (Intern), Ovtar, S. (Intern), Tripkovic, D. (Intern)
Publication date: 2017
Conference: 231st ECS Meeting, New Orleans, LA, United States, 28/05/2017 - 28/05/2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Electrochemical Society. Meeting Abstracts (Online)
Volume: MA2017-01
Article number: 1581
ISSN (Print): 2151-2043
Original language: English
Links:
http://ma.ecsdl.org/content/MA2017-01/33/1581.abstract

Publication: Research - peer-review › Conference abstract in journal – Annual report year: 2017

Ion-Exchange-Induced Selective Etching for the Synthesis of Amino-Functionalized Hollow Mesoporous Silica for Elevated-High-Temperature Fuel Cells

As differentiated from conventional synthetic processes, amino-functionalized hollow mesoporous silica (NH$_2$–HMS) has been synthesized using a new and facile strategy of ion-exchange-induced selective etching of amino-functionalized mesoporous silica (NH$_2$–meso-silica) by an alkaline solution. Nuclear magnetic resonance (NMR) spectroscopy and in situ time-resolved small-angle X-ray scattering (SAXS) reveal that ion-exchange-induced selective etching arises from the gradient distribution of OH$^-$ in the NH$_2$–meso-silica nanospheres. Moreover, the ion-exchange-induced selective etching mechanism is verified through a successful synthesis of hollow mesoporous silica. After infiltration with phosphotungstic acid (PWA), PWA–NH$_2$–HMS nanoparticles are dispersed in the poly(ether sulfone)–polyvinylpyrrolidone (PES–PVP) matrix, forming a hybrid PWA–NH$_2$–HMS/PES–PVP nanocomposite membrane. The resultant nanocomposite membrane with an optimum loading of 10 wt% of PWA–NH$_2$–HMS showed an enhanced proton conductivity of 0.175 S cm$^{-1}$ and peak power density of 420 mW cm$^{-2}$ at 180 °C under anhydrous conditions. Excellent durability of the hybrid composite membrane fuel cell has been demonstrated at 200 °C. The results of this study demonstrated the potential of the facile synthetic strategy in the fabrication of NH$_2$–HMS with controlled mesoporous structure for application in nanocomposite membranes as a technology platform for elevated-temperature proton exchange membrane fuel cells.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors, Curtin University, Deakin University, Beihang University
Ionic/Electronic Conductivity, Thermal/Chemical Expansion and Oxygen Permeation in Pr and Gd Co-Doped Ceria $\text{Pr}_x\text{Gd}_{0.1}\text{Ce}_{0.9-x}\text{O}_{1.95-\delta}$

The oxygen permeation flux of $\text{Ce}_0\text{Gd}_{0.1}\text{O}_{1.95-\delta}$ (CGO)-based oxygen transport membranes under oxidizing conditions is limited by the electronic conductivity of the material. This work aims to enhance the bulk ambipolar conductivity of CGO by partial substitution of Ce with the redox active element Pr. A series of compositions of $\text{Pr}_x\text{Gd}_{0.1}\text{Ce}_{0.9-x}\text{O}_{1.95-\delta}$ ($x = 0, 0.02, 0.05, 0.08, 0.15, 0.25, 0.3$ and $0.4$) was prepared by solid state reaction. X-ray powder diffraction (XPD) indicates that Pr is completely dissolved in the fluorite structure up to $40\text{ at.%). Pronounced nonlinear thermal expansion behavior was observed as a function of temperature, due to the simultaneous contributions of both thermal and chemical expansion. The electronic and ionic conductivities were measured as a function of temperature and oxygen partial pressure. Within the range from $10$ to $15\text{ at.\% Pr}$, a drastic drop of the activation energy of the hole mobility and an abrupt increase of the hole conductivity at low temperature was observed. The behavior could be rationalized by a simple percolation model. Oxygen permeation fluxes through disk shaped samples fed with air on one side and $\text{N}_2$ on the other side were also measured. The oxygen flux through $\text{Pr}_{0.05}\text{Gd}_{0.1}\text{Ce}_{0.85}\text{O}_{1.95-\delta}$ was higher than that for CGO by one order
of magnitude owing to the enhanced electronic conductivity albeit the flux is still limited by the electronic conductivity. In terms of the electronic and ionic conductivity, the estimated maximum oxygen permeation flux of a 10 μm Pr$_{0.4}$Gd$_{0.1}$Ce$_{0.9}$O$_{1.95-δ}$-based membrane exceeds 10 NmL cm$^{-2}$ min$^{-1}$ at 900°C under a small oxygen potential gradient (0.21/10$^{-3}$ bar) which is promising for use in oxygen production and in oxy-fuel combustion. Also the material may be well applicable to SOFC/SOEC composite electrodes where mixed conductivity is also desirable.

**General information**

State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Mixed Conductors
Authors: Cheng, S. (Intern), Chatzichristodoulou, C. (Intern), Søgaard, M. (Intern), Kaiser, A. (Intern), Hendriksen, P. V. (Intern)
Pages: F1354-F1367
Publication date: 2017
Main Research Area: Technical/natural sciences

**Publication information**

Journal: Journal of the Electrochemical Society
Volume: 164
Issue number: 13
ISSN (Print): 0013-4651
Ratings:
- BFI (2018): BFI-level 1
- Web of Science (2018): Indexed yes
- BFI (2017): BFI-level 1
- Scopus rating (2017): CiteScore 3.48 SJR 1.267 SNIP 1.009
- Web of Science (2017): Indexed yes
- BFI (2016): BFI-level 1
- Scopus rating (2016): CiteScore 2.97 SJR 1.222 SNIP 0.963
- Web of Science (2016): Indexed yes
- BFI (2015): BFI-level 1
- Scopus rating (2015): SJR 1.115 SNIP 1.066 CiteScore 3.17
- Web of Science (2015): Indexed yes
- BFI (2014): BFI-level 1
- Scopus rating (2014): SJR 1.213 SNIP 1.25 CiteScore 3.36
- Web of Science (2014): Indexed yes
- BFI (2013): BFI-level 1
- Scopus rating (2013): SJR 1.169 SNIP 1.309 CiteScore 2.92
- ISI indexed (2013): ISI indexed yes
- Web of Science (2013): Indexed yes
- BFI (2012): BFI-level 1
- Scopus rating (2012): SJR 1.329 SNIP 1.281 CiteScore 2.61
- ISI indexed (2012): ISI indexed yes
- Web of Science (2012): Indexed yes
- BFI (2011): BFI-level 1
- Scopus rating (2011): SJR 1.331 SNIP 1.335 CiteScore 2.74
- ISI indexed (2011): ISI indexed yes
- Web of Science (2011): Indexed yes
- BFI (2010): BFI-level 1
- Scopus rating (2010): SJR 1.418 SNIP 1.304
- Web of Science (2010): Indexed yes
- BFI (2009): BFI-level 1
- Scopus rating (2009): SJR 1.442 SNIP 1.27
- Web of Science (2009): Indexed yes
- BFI (2008): BFI-level 1
- Scopus rating (2008): SJR 1.595 SNIP 1.41
- Web of Science (2008): Indexed yes
- Scopus rating (2007): SJR 1.569 SNIP 1.322
Is γ-Al₂O₃ polar?

Polarity in thin films and polar discontinuities across an interface plays an important role in determining electronic properties. A key example is the conductivity at the LaAlO₃/SrTiO₃ (LAO/STO) interface, which is proposed to originate from the polarity of LAO. As a consequence, the conductivity does not disappear when LAO/STO is subjected to highly oxidizing conditions. Substituting LAO with another nominally polar material γ-Al₂O₃ (GAO) results in an interface conductivity which can be destroyed by annealing in oxygen. We investigate this apparent paradox by revisiting the defect spinel atomic structure of GAO. We show that the polarity is dependent on the distribution of aluminum vacancies which are intrinsically present in GAO to ensure charge neutrality. In particular, certain film thicknesses allow for vacancy distributions that make GAO nominally non-polar along the [001] direction. We further propose that electromigration of aluminum vacancies across atomic layers can alter the polarity, making the GAO film effectively act as a ferroelectric.
Jahn-Teller and Non-Jahn-Teller Systems Involving CuF\textsubscript{6}\textsuperscript{4−} Units: Role of the Internal Electric Field in Ba\textsubscript{2}ZnF\textsubscript{6}:Cu\textsuperscript{2+} and Other Insulating Systems

The applicability of the Jahn-Teller (JT) framework to 6-fold coordinated d\textsuperscript{9} ions whose local symmetry is not strictly octahedral is explored by means of first principle calculations. Our results contradict much of the existing literature where these systems are analyzed within the quasi-JT regime which assumes the usual JT description with a small splitting between b\textsubscript{1g} (\(\sim x^2-y^2\)) and a\textsubscript{1g} (\(\sim 3z^2-r^2\)) orbitals and also the existence of three nearly equivalent distortions. To clarify this issue we investigate the equilibrium geometry (equatorial, R\textsubscript{eq}, and axial, R\textsubscript{ax}, Cu\textsuperscript{2+}-F\textsuperscript{−} distances) and optical
transitions for CuF$_6^{4-}$ units formed in Cu$^{2+}$-doped the tetragonal Ba$_2$ZnF$_6$ host lattice. While the experimental d-d transitions cannot be reproduced through the isolated CuF$_6^{4-}$ unit at the equilibrium geometry, a reasonable agreement is reached adding in the calculation the internal electric field, $E_R(r)$, created by the rest of lattice ions on the electrons confined in the complex. It is shown that this tetragonal field, $E_R(r)$, already produces a gap $\Delta_0 \sim 0.35$ eV between $b_1g$ ($\sim x^2-y^2$) and $a_1g$ ($\sim 3z^2-r^2$) orbitals of Ba$_2$ZnF$_6$.Cu$^{2+}$ when $R_{ax} = R_{eq}$. Nevertheless, as this internal field leads to a $\Delta_0$ value higher than typical JT barriers it drastically modifies the characteristic pattern of a JT effect. In particular, it prevents the existence of three equivalent distortions as confirmed by experimental EPR data. Furthermore, $E_R(r)$ is shown to be the main physical reason behind an unusual compressed ground state with the hole in the $a_{1g}$ ($\sim 3z^2-r^2$) level while it is always placed in the $b_{1g}$ ($\sim x^2-y^2$) level for MX$_6$ complexes (M = Cu$^{2+}$, Ag$^{2+}$, Ni$^{2+}$; X = F$^-$, Cl$^-$) in cubic lattices displaying a static JT effect. While the experimental results of CuF$_6^{4-}$ in Ba$_2$ZnF$_6$ cannot be understood within the JT framework it is pointed out that a quasi-JT situation can however happen for a d$^9$ ion in a cubic lattice under a strain of $\sim 10^{-3}$ in agreement with experimental data. The present results stress the key role played by the internal electric fields for a quantitative understanding of compounds with transition metal cations. Moreover, they also demonstrate that in the interpretation of experimental data the use of a simple model should be avoided unless all its assumptions are well justified.

**General information**

State: Published
Organisations: Atomic scale modelling and materials, Theoretical Atomic-scale Physics, Universidad de Cantabria
Authors: Aramburu, J. A. (Ekstern), Garcia-Fernandez, P. (Ekstern), García Lastra, J. M. (Intern), Moreno, M. (Ekstern)
Number of pages: 10
Pages: 5215-5224
Publication date: 2017
Main Research Area: Technical/natural sciences

**Publication information**

Journal: Journal of Physical Chemistry C
Volume: 121
Issue number: 9
ISSN (Print): 1932-7447
Ratings:
- BFI (2018): BFI-level 1
- Web of Science (2018): Indexed yes
- BFI (2017): BFI-level 1
- Scopus rating (2017): CiteScore 4.58 SJR 2.135 SNIP 1.147
- Web of Science (2017): Indexed yes
- BFI (2016): BFI-level 1
- Scopus rating (2016): CiteScore 4.48 SJR 1.964 SNIP 1.195
- Web of Science (2016): Indexed yes
- BFI (2015): BFI-level 1
- Scopus rating (2015): SJR 1.886 SNIP 1.26 CiteScore 4.68
- Web of Science (2015): Indexed yes
- BFI (2014): BFI-level 1
- Scopus rating (2014): SJR 2.032 SNIP 1.447 CiteScore 5.08
- Web of Science (2014): Indexed yes
- BFI (2013): BFI-level 1
- Scopus rating (2013): SJR 2.143 SNIP 1.445 CiteScore 5.14
- ISI indexed (2013): ISI indexed yes
- Web of Science (2013): Indexed yes
- BFI (2012): BFI-level 1
- Scopus rating (2012): SJR 2.529 SNIP 1.461 CiteScore 4.98
- ISI indexed (2012): ISI indexed yes
- Web of Science (2012): Indexed yes
- BFI (2011): BFI-level 1
- Scopus rating (2011): SJR 2.339 SNIP 1.465 CiteScore 4.92
- ISI indexed (2011): ISI indexed yes
- Web of Science (2011): Indexed yes
- BFI (2010): BFI-level 1
- Scopus rating (2010): SJR 2.462 SNIP 1.362
Large Differences in the Optical Spectrum Associated with the Same Complex: The Effect of the Anisotropy of the Embedding Lattice

Transition-metal complexes with a well-defined geometry are usually considered to display almost the same properties independently of the system where they are embedded. Here we show that the above statement is not true depending on the anisotropy of the host lattice, which is revealed in the form of the electric field created by the rest of lattice ions over the complex. To illustrate this concept we analyze the origin of the surprisingly large differences in the $d$–$d$ optical transitions of two systems containing square-planar CuF$_4^{2-}$ complexes, CaCuF$_4$, and center II in Cu$^{2+}$–doped Ba$_2$ZnF$_6$, even though the Cu$^{2+}$–F distance difference is just found to be 1%. Using a minimalist first-principles model we show that the different morphology of the host lattices creates an anisotropic field that red-shifts the in vacuo complex transitions to the 1.25–1.70 eV range in CaCuF$_4$, while it blue-shifts them to the 1.70–3.0 eV region in Ba$_2$ZnF$_6$:Cu$^{2+}$. This particular example shows how the lattice anisotropy strongly alters the optical properties of a given transition-metal complex. This knowledge opens a new path to tune the spectra of this large family of systems.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, Universidad de Cantabria
Authors: Aramburu, J. A. (Ekstern), García-Fernández, P. (Ekstern), García Lastra, J. M. (Intern), Moreno, M. (Ekstern)
Number of pages: 10
Pages: 8944-8953
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Inorganic Chemistry
Volume: 56
Issue number: 15
ISSN (Print): 0020-1669
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 4.7 SJR 1.892 SNIP 1.123
Web of Science (2017): Indexed Yes
Lattice constant measurement from electron backscatter diffraction patterns

Kikuchi bands in electron backscattered diffraction patterns (EBSP) contain information about lattice constants of crystallographic samples that can be extracted via the Bragg equation. An advantage of lattice constant measurement from EBSPs over diffraction (XRD) is the ability to perform local analysis. In this study, lattice constants of cubic STN and cubic YSZ in the pure materials and in co-sintered composites were measured from their EBSPs acquired at 10 kV using a silicon single crystal as a calibration reference. The EBSP distortion was corrected by spherical back projection and Kikuchi band analysis was made using in-house software. The error of the lattice constant measurement was determined to be in the range of 0.09–1.12% compared to values determined by XRD and from literature. The confidence level of the method is indicated by the standard deviation of the measurement, which is approximately 0.04 Å. Studying Kikuchi band size dependence of the measurement precision shows that the measurement error decays with increasing band size (i.e. decreasing lattice constant). However, in practice, the sharpness of wide bands tends to be low due to their low intensity, thus limiting the measurement precision. Possible methods to improve measurement precision are suggested.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Imaging and Structural Analysis
Authors: Saowadee, N. (Intern), Agersted, K. (Ekstern), Bowen, J. R. (Intern)
Pages: 200-210
Publication date: 2017
Main Research Area: Technical/natural sciences

Publications information
Journal: Journal of Microscopy
Volume: 266
Issue number: 2
ISSN (Print): 0022-2720
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 0.94 SJR 0.728 CiteScore 1.85
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.9 SJR 0.746 SNIP 0.841
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.962 SNIP 1.095 CiteScore 2.37
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.067 SNIP 1.339 CiteScore 2.41
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.749 SNIP 1.051 CiteScore 1.96
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.764 SNIP 1.276 CiteScore 1.84
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.873 SNIP 0.918 CiteScore 1.67
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.962 SNIP 0.963
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.786 SNIP 0.881
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.737 SNIP 1.034
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.968 SNIP 1.04
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.068 SNIP 1.128
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.172 SNIP 1.146
Scopus rating (2004): SJR 1.202 SNIP 1.24
Scopus rating (2003): SJR 1.149 SNIP 1.392
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 1.093 SNIP 1.105
Scopus rating (2001): SJR 1.021 SNIP 1.241
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 0.712 SNIP 1.13
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 0.833 SNIP 0.948
Original language: English
EBSD, EBSD pattern, Kikuchi band width, Lattice constant, Strontium titanate, XRD, Yttria-stabilized zirconia
Electronic versions:
Saowadee_et_al_Lattice_constants_from_EBSD_post_print.pdf. Embargo ended: 19/04/2018
DOIs:
10.1111/jmi.12529
Publication: Research - peer-review › Journal article – Annual report year: 2017

**Lead-free, textured piezoelectric ceramics**

*General information*
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Universite Francois Rabelais, Meggitt A/S
Authors: Bjørnetun Haugen, A. (Intern), Ringgaard, E. (Ekstern), Levarssort, F. (Ekstern)
Number of pages: 1
Publication date: 2017

*Host publication information*
Title of host publication: Book of Abstracts, Sustain 2017
Publisher: Technical University of Denmark (DTU)
Article number: M-23
Main Research Area: Technical/natural sciences
Conference: Sustain 2017, Kgs. Lyngby, Denmark, 06/12/2017 - 06/12/2017
Electronic versions:
SustainAbstracts2017c.compressed_133.pdf
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2017

**Life cycle assessment of hydrogen production from water electrolysis**

*General information*
State: Published
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry, Mixed Conductors, Proton conductors
Number of pages: 1
Publication date: 2017

*Host publication information*
Title of host publication: Book of Abstracts, Sustain 2017
Publisher: Technical University of Denmark (DTU)
Article number: M-12
Life-Cycle Assessment of Solar Charger with Integrated Organic Photovoltaics

Organic photovoltaics (OPV) applied in a commercial product comprising a solar charged power bank is subjected to a life cycle assessment (LCA) study. Regular power banks harvest electricity from the grid only. The solar power bank (called HeLi-on) is however, a power bank that includes a portable OPV panel, enabling the possibility to be charged from the sun, and not only from the grid. In this paper, two well-established power bank products using amorphous silicon solar panels (a-Si PV) and a regular power bank without any portable solar panel is compared to HeLi-on. The environmental impact of the products is quantified with the aim of indicate where eco-design improvements would make a difference and to point out performance of a portable solar panel depending on the context of use (Denmark and China), realistic disposal scenarios and the recycling relevance particularly concerning metals content.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Organic Energy Materials
Authors: Benatto, G. A. D. R. (Intern), Espinosa Martinez, N. (Intern), Krebs, F. C. (Intern)
Number of pages: 7
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Advanced Engineering Materials
Volume: 19
Issue number: 8
Article number: 1700124
ISSN (Print): 1438-1656
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SJR 0.924 SNIP 1.116 CiteScore 2.47
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.07 SJR 0.834 SNIP 1.125
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.806 SNIP 1.028 CiteScore 1.82
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.802 SNIP 1.055 CiteScore 1.66
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.737 SNIP 0.84 CiteScore 1.59
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.778 SNIP 0.951 CiteScore 1.46
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.836 SNIP 1.03 CiteScore 1.58
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.098 SNIP 1.151
Lifetime limiting effects in pre-commercial solid oxide cell devices

The solidoxide electrochemical cell technology is promising for efficient energy storage, especially when the share of intermittent renewable electricity production is high. The technology is being commercialized in niche markets, but large-scale employments still hindered by limited durability of the devices. The lifetime limiting mechanisms are addressed in this work.

A general introduction into mechanisms limiting the durability is presented. A database of more than 50 parameters from 150 publications and 1,000,000 hours of accumulated testing was established, and a quantitative analysis of degradation and lifetime was conducted. It is shown that the technology is approaching the official targets required for commercialization, but that work remains to be done.

It is further recognized that targeting niche applications initially will allow for employment of economies of scale, which will bring down costs and facilitate entry into larger markets. Here, we examine electrochemical reduction of CO2 to CO and one of the main failure mechanisms related to it. Carbon formation on the nickel electrocatalyst can be detrimental to the microstructural integrity of the cell. It is found that the possible operating window is severely limited due to gradients of temperature, gas concentration and overpotential across the electrode. These affects also apply to stack- and system-level, and the results obtained are combined with modeling and stack testing experiences. Thus, on account of this mechanism the possible outlet CO concentration is limited by up to 50% below the thermodynamic carbon deposition threshold based on the inlet temperature, depending on design and operating strategy.

Replacement of the Ni electrocatalyst would increase the stability towards this issue and may improve the robustness in other ways as well. Cerihas been reported as a potential candidate in such endeavors. Thin film electrodes of nickel and ceria are therefore studied as model systems using near-ambient pressure x-ray photoelectron spectroscopy to further the fundamental understanding of the carbon formation mechanism. The reaction occurs further from the thermodynamic threshold on ceria, and fundamental mechanisms for electrochemically driven carbon growth are suggested based on observed adsorbate species.

By infiltrating ceria after degradation has already occurred, the robustness and lifetime of the cells are increased. Complete reactivation of the fuel electrode is achieved after otherwise detrimental failure mechanisms have occurred, such as reactant starvation and carbon formation. Moreover, the degradation of the electrode over the course of nearly 2500 hours is essentially eliminated by infiltrating after microstructural stabilization had occurred. Lastly, the method is scaled up by replicating the positive effects of post-degradation infiltration on an 8-cell stack.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry
Authors: Skafte, T. L. (Intern), Hjelm, J. (Intern), Graves, C. R. (Intern)
Number of pages: 142
Publication date: 2017
Lithium-Oxygen Batteries: At a Crossroads?
In this current opinion, we critically review and discuss some of the most important recent findings in the field of rechargeable lithium-oxygen batteries. We discuss recent discoveries like the evolution of reactive singlet oxygen and the use of organic additives to bypass reactive LiO2 reaction intermediates, and their possible implications on the potential for commercialization of lithium-oxygen batteries. Finally, we perform a critical assessment of lithium-superoxide batteries and the reversibility of lithium-hydroxide batteries.

Long-term durability of HT-PEM fuel cells based on thermally crosslinked polybenzimidazole
Long-term durability of HT-PEM fuel cells based on thermally crosslinked polybenzimidazole

Publication information
Publisher: Department of Energy Conversion and Storage, Technical University of Denmark
Original language: English
Main Research Area: Technical/natural sciences

Relations
Projects:
Lifetime limiting effects in pre-commercial solid oxide cell devices
Publication: Research › Ph.D. thesis – Annual report year: 2017

Lithium-Oxygen Batteries: At a Crossroads?
In this current opinion, we critically review and discuss some of the most important recent findings in the field of rechargeable lithium-oxygen batteries. We discuss recent discoveries like the evolution of reactive singlet oxygen and the use of organic additives to bypass reactive LiO2 reaction intermediates, and their possible implications on the potential for commercialization of lithium-oxygen batteries. Finally, we perform a critical assessment of lithium-superoxide batteries and the reversibility of lithium-hydroxide batteries.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, University of Michigan-Dearborn
Authors: Vegge, T. (Intern), García Lastra, J. M. (Intern), Siegel, D. J. (Intern)
Pages: 100-107
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Current Opinion in Electrochemistry
Volume: 6
Issue number: 1
ISSN (Print): 2451-9103
Original language: English
DOIs:
10.1016/j.coelec.2017.10.014
Publication: Research - peer-review › Journal article – Annual report year: 2017

Long-term durability of HT-PEM fuel cells based on thermally crosslinked polybenzimidazole
Long-term durability of HT-PEM fuel cells based on thermally crosslinked polybenzimidazole

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors, Danish Power Systems ApS
Authors: Søndergaard, T. (Intern), Cleemann, L. N. (Intern), Becker, H. (Intern), Aili, D. (Intern), Steenberg, T. (Ekstern), Hjuler, H. A. (Ekstern), Seerup, L. (Intern), Li, Q. (Intern), Jensen, J. O. (Intern)
Pages: 570-578
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Power Sources
Volume: 342
ISSN (Print): 0378-7753
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 7 SJR 2.202 SNIP 1.536
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 6.22 SJR 1.944 SNIP 1.5
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Long Term Testing of Solid Oxide Electrolysis Cells under Co-Electrolysis Conditions

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry
Authors: Rao, M. (Intern), Sun, X. (Intern), Hagen, A. (Intern)
Pages: 1
Publication date: 2017
Conference: 232nd ECS meeting, National Harbor, Washington, DC, United States, 01/10/2017 - 01/10/2017

Original language: English
Durability, Polymer electrolyte membrane, Fuel cell, Polybenzimidazole, Cross-linking, Thermally cured

DOIs: 10.1016/j.jpowsour.2016.12.075
Source: PublicationPreSubmission
Source-ID: 128050356
Publication: Research - peer-review › Journal article – Annual report year: 2017
Long Term Testing of Solid Oxide Electrolysis Cells Under Co-Electrolysis Conditions

SOECs consisting of a nickel-yttria stabilized zirconia (Ni-YSZ) fuel electrode, YSZ electrolyte and lanthanum strontium cobalt ferrite-gadolinium doped ceria (LSCF-GDC) composite oxygen electrode were tested under co-electrolysis (H₂O+CO₂) conditions. The aim in this study was to compare the SOEC durability under co-electrolysis conditions between galvanostatic and potentiostatic modes. Specifically, the cells were operated at 0.75 A/cm² (galvanostatic) and at 1.2 V (potentiostatic) at 750 °C for over 1000 hours. In both modes, a larger degradation was observed initially for the first 200 hours of testing, followed by a more stable performance over longer operating times. Trends of the area specific resistance (ASR) and detailed electrochemical analysis of the cell’s performance under durability conditions for both modes indicated that the degradation was predominantly due to the fuel electrode along with a slight contribution from the oxygen electrode. Microstructural analysis also confirmed the degradation of the active fuel electrode.
Low surface damage dry etched black silicon

Black silicon (bSi) is promising for integration into silicon solar cell fabrication flow due to its excellent light trapping and low reflectance, and a continuously improving passivation. However, intensive ion bombardment during the reactive ion etching used to fabricate bSi induces surface damage that causes significant recombination. Here, we present a process optimization strategy for bSi, where surface damage is reduced and surface passivation is improved while excellent light trapping and low reflectance are maintained. We demonstrate that reduction of the capacitively coupled plasma power, during reactive ion etching at non-cryogenic temperature (-20°C), preserves the reflectivity below 1% and improves the effective minority carrier lifetime due to reduced ion energy. We investigate the effect of the etching process on the surface morphology, light trapping, reflectance, transmittance, and effective lifetime of bSi. Additional surface passivation using atomic layer deposition of Al2O3 significantly improves the effective lifetime. For n-type wafers, the lifetime reaches 12 ms for polished and 7.5 ms for bSi surfaces. For p-type wafers, the lifetime reaches 800 ls for both polished and bSi surfaces.
Low Temperature Synthesis and Properties of Gadolinium-Doped Cerium Oxide Nanoparticles

Gadolinium-doped cerium oxide (GDC) is an attractive ceramic material for solid oxide fuel cells (SOFCs) both as the electrolyte and in composite electrodes operating at low and intermediate temperatures. GDC exhibits high oxygen ion conductivity at a wide range of temperatures and displays a high resistance to carbon deposition when hydrocarbons are used as fuels. However, an inconvenience of ceria-based oxides is the high sintering temperature needed to obtain a fully dense ceramic body. In this study, a green chemistry route for the synthesis of 10 mol% GDC nanoparticles is proposed. The aqueous precipitation method starts from the nitrates of both cerium and gadolinium and uses excess hexamethylenetetramine (HMT) to produce crystalline GDC at 80°C. Such a low temperature synthesis provides control over particle size and sinterability of the material at low temperatures.
Low Temperature Synthesis and Properties of Gadolinium-Doped Cerium Oxide Nanoparticles

Gadolinium-doped cerium oxide (GDC) is an attractive ceramic material for solid oxide fuel cells (SOFCs) both as the electrolyte or in composite electrodes. The Ni/GDC cermet can be tuned as a catalytic layer, added to the conventional Ni/yttria-stabilized zirconia (YSZ), for the internal steam reforming of different fuels. Such an anode allows the SOFC to operate with hydrocarbon fuels by internal reforming. GDC exhibits high oxygen ion conductivity at a wide range of temperatures and displays a high resistance to carbon deposition. However, an inconvenience of ceria-based oxides is the high sintering temperature needed to obtain a fully dense ceramic body, which can result in undesired reactions with YSZ.

In this study, a green chemistry route for the synthesis of 10 mol% GDC nanoparticles is proposed. Such a low temperature synthesis provides control over particle size and sinterability of the material. The aqueous precipitation method starts from the nitrates of both cerium and gadolinium and uses excess hexamethylenetetramine (HMT) to produce crystalline GDC at 80 °C. As-produced powders were found to be GDC crystalline fluorite-type structure, with
crystallite size ≤ 10 nm. Thermal gravimetric analysis show a small mass loss and dilatometry profiles show a total retraction of > 20% up to 1400 °C. The electrical properties of the material were studied by impedance spectroscopy measurements of sintered samples in a controlled atmosphere. The samples sintered for 2 hours at 1400 °C exhibited electrical conductivity comparable to previously reported data for GDC.

**General information**
- **State**: Published
- **Organisations**: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Instituto de Pesquisas Energeticas e Nucleares, Universidade Federal do ABC
- **Authors**: Machado, M. F. S. (Ekstern), P. R. Moraes, L. (Ekstern), Monteiro, N. K. (Ekstern), Esposito, V. (Intern), Zanetti De Florio, D. (Ekstern), Marani, D. (Intern), C. Fonseca, F. (Ekstern)
- **Pages**: 1
- **Publication date**: 2017
- **Conference**: 15th International Symposium on Solid Oxide Fuel Cells (SOFC-XV), Hollywood, United States, 23/07/2017 - 23/07/2017
- **Main Research Area**: Technical/natural sciences

**Publications information**
- **Journal**: Electrochemical Society. Meeting Abstracts (Online)
- **Volume**: MA2017-03
- **Article number**: 322
- **ISSN (Print)**: 2151-2043
- **Original language**: English
- **Links**:
  - http://ma.ecsdl.org.proxy.findit.dtu.dk/content/MA2017-03/1/322.abstract
- **Publication**: Research - peer-review › Conference abstract in journal – Annual report year: 2017

Luminescence Imaging Strategies for Drone-Based PV Array Inspection

The goal of this work is to develop outdoor defect detection imaging and understand fully its challenges and limitations. The imaging is based on luminescence strategies that will be used for fast and accurate UAV-based inspection system for PV power plants. We studied electroluminescence (EL) acquisition under natural light conditions during several times of the day, under high sun irradiation, to unveil the sunlight noise characteristics towards an InGaAs detector. In order to bring more freedom to a drone-based inspection, we also show the preliminary results of a laser-line based photoluminescence (PL) strategy as a viable method for an outdoor module PL imaging system.

**General information**
- **State**: Published
- **Organisations**: Department of Photonics Engineering, Photovoltaic Materials and Systems, Organic Energy Materials, Coding and Visual Communication, Diode Lasers and LED Systems
- **Number of pages**: 5
- **Publication date**: 2017

**Host publication information**
- **Title of host publication**: Proceedings of 33rd European Photovoltaic Solar Energy Conference and Exhibition
- **Main Research Area**: Technical/natural sciences
- **Conference**: 33rd European Photovoltaic Solar Energy Conference and Exhibition Amsterdam, Netherlands, 25/09/2017 - 25/09/2017
- **Electroluminescence, Photoluminescence, Defects, Inspections**

**Relations**
- **Projects**: Luminescence Imaging Strategies for Drone-Based PV Array Inspection

**Magnetic two-dimensional electron gas at the manganite-buffered LaAlO3/SrTiO3 interface**

Fabrication of highly mobile spin-polarized two-dimensional electron gas (2DEG) is crucially important for both fundamental and applied research. Usually, spin polarization appears below 10 K for the 2DEG of LaAlO3/SrTiO3 interface, stemming from the magnetic ordering of Ti3+ ions with the mediation of itinerant electrons. Herein, we report a magnetic 2DEG at a La7/8Sr1/8MnO3-buffered LaAlO3/SrTiO3 interface, which simultaneously shows electrically tunable anomalous Hall effect and high conductivity. The spin-polarized temperature for the 2DEG is promoted to 30 K while the
mobility remains high. The magnetism likely results from a gradient manganese interdiffusion into SrTiO3. The present work demonstrates the great potential of manganite-buffered LaAlO3/SrTiO3 interfaces for spintronic applications.

**General information**

**State:** Published

**Organisations:** Department of Energy Conversion and Storage, Electrofunctional materials, Chinese Academy of Sciences

**Authors:** R. Zhang, H. (Ekstern), Zhang, Y. (Ekstern), Zhang, H. (Ekstern), Zhang, J. (Ekstern), Shen, X. (Ekstern), Guan, X. X. (Ekstern), Chen, Y. (Intern), Yu, R. C. (Ekstern), Pryds, N. (Intern), Chen, Y. S. (Ekstern), Shen, B. G. (Ekstern), Sun, J. R. (Ekstern)

**Number of pages:** 7

**Publication date:** 2017

**Main Research Area:** Technical/natural sciences

**Publication information**

**Journal:** Physical Review B

**Volume:** 96

**Issue number:** 19

**Article number:** 195167

**ISSN (Print):** 2469-9950

**Ratings:**

- BFI (2018): BFI-level 1
- Web of Science (2018): Indexed yes
- BFI (2017): BFI-level 2
- Scopus rating (2017): CiteScore 3.34 SJR 1.604 SNIP 1.04
- Web of Science (2017): Indexed yes
- Scopus rating (2016): CiteScore 3.16 SJR 2.339 SNIP 1.151
- Web of Science (2016): Indexed yes
- Scopus rating (2015): SJR 2.377 SNIP 1.13 CiteScore 2.8
- Web of Science (2015): Indexed yes
- Scopus rating (2014): SJR 2.762 SNIP 1.316 CiteScore 3.3
- Web of Science (2014): Indexed yes
- Scopus rating (2013): SJR 2.813 SNIP 1.326 CiteScore 3.55
- ISI indexed (2013): ISI indexed yes
- Web of Science (2013): Indexed yes
- Scopus rating (2012): SJR 3.173 SNIP 1.378 CiteScore 3.57
- ISI indexed (2012): ISI indexed yes
- Web of Science (2012): Indexed yes
- Scopus rating (2011): SJR 3.326 SNIP 1.423 CiteScore 3.61
- ISI indexed (2011): ISI indexed yes
- Web of Science (2011): Indexed yes
- Scopus rating (2010): SJR 3.318 SNIP 1.447
- Web of Science (2010): Indexed yes
- Web of Science (2009): Indexed yes
- Scopus rating (2008): SJR 2.923 SNIP 1.516
- Web of Science (2008): Indexed yes
- Scopus rating (2007): SJR 2.892 SNIP 1.588
- Web of Science (2007): Indexed yes
- Scopus rating (2006): SJR 2.62 SNIP 1.468
- Web of Science (2006): Indexed yes
- Scopus rating (2005): SJR 2.126 SNIP 1.156
- Web of Science (2005): Indexed yes
- Scopus rating (2004): SJR 2.012 SNIP 1.103
- Web of Science (2004): Indexed yes
- Scopus rating (2003): SJR 2.184 SNIP 1.179
- Web of Science (2003): Indexed yes
- Scopus rating (2002): SJR 2.856 SNIP 1.841
Materials for Catalysis, Synthetic Fuels and Chemical Energy Conversion

General information
State: Published
Organisations: Department of Energy Conversion and Storage
Authors: Joya, K. S. (Intern), Kammer Hansen, K. (Intern), Holtappels, P. (Intern)
Number of pages: 1
Publication date: 2017

Host publication information
Title of host publication: Book of Abstracts Sustain 2017
Article number: C-1
Main Research Area: Technical/natural sciences
Conference: Sustain 2017, Kgs. Lyngby, Denmark, 06/12/2017 - 06/12/2017
Electronic versions:
SustainAbstracts2017c.compressed_16.pdf
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2017

Mechanical Investigation of Various Stack Designs for Solid Oxide Cells

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, University of Central Florida
Authors: Tadesse Molla, T. (Intern), Kwok, K. (Ekstern), Frandsen, H. L. (Intern)
Number of pages: 1
Publication date: 2017

Host publication information
Title of host publication: ECS Meeting Abstracts
Volume: MA2017-03
Publisher: The Electrochemical Society
Article number: 181
Main Research Area: Technical/natural sciences
Conference: 15th International Symposium on Solid Oxide Fuel Cells (SOFC-XV), Hollywood, United States, 23/07/2017 - 23/07/2017
Solid oxide fuel cells, Metallic interconnect, Creep, Finite element modeling
Links:
http://ma.ecsdl.org.proxy.findit.dtu.dk/content/MA2017-03/1/181
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2017

Mechanical properties of biaxially strained poly(L-lactide) tubes: Strain rate and temperature dependence
Poly(l-lactide) (PLLA) is a bioabsorbable polymer with high stiffness and strength compared to the other commercially available bioabsorbable polymers. The properties of PLLA can be improved by straining, causing deformation-mediated molecular orientation. PLLA tubes were biaxially strained above their $T_g$ for improvement of their strength, in a two-step process (sequential straining). Mechanical properties and crystal morphology were investigated as a function of processing strain rate and temperature. DSC revealed that a low processing strain rate allows molecular chain relaxation in the direction of strain and the crystallization is suppressed. Faster strain rates on the other hand suppress chain relaxation, and results in crystalline tubes. The mechanical properties are influenced by both processing strain rate and
temperature. Low strain rates allow chain relaxation resulting in the lowest strength and stiffness, whereas a larger stiffness and strength is achieved by increasing strain rate and temperature. Isotropic mechanical properties are only observed at high processing strain rates.
Mechanical Properties of Supports and Half-Cells for Solid Oxide Electrolysis Influenced by Alumina-Zirconia Composites

In order to improve the durability and robustness of solid oxide electrolysis cells (SOEC) and stacks, it is necessary to improve the strength of its components. In cathode supported SOEC, the main structural component is the Ni(O)-YSZ support. But the strength of the half-cell or cell is also determined by the strength of other weaker components and by the residual stress state induced by the thermal expansion mismatch. In this study, the mechanical properties of Ni(O)-3YSZ supports with a reference composition and with substitution of 3YSZ by 20A3YSZ (3YSZ with 20 wt.% Al2O3) have been tested and compared. The initial interest of this substitution are a decrease of the coefficient of thermal expansion (CTE) mismatch within the half-cell and the fact that 20A3YSZ is stronger than 3YSZ. The influence of the process on the composition, strength, elastic properties and electrical conductivity of the supports have been measured and analyzed. The short and long-term evolution of these properties is linked to the formation of a NiAl2O4 phase. The samples properties were measured at room temperature or high temperature (800 °C) and in oxidized or reduced conditions. The impact of these supports on residual stresses and strength of half-cells is also discussed.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Ceramic Engineering & Science
Authors: Charlas, B. (Intern), Ni, D. W. (Intern), Frandsen, H. L. (Intern), Brodersen, K. (Intern), Chen, M. (Intern)
Pages: 132-143
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Fuel Cells
Volume: 17
Issue number: 2
ISSN (Print): 1615-6846
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 1.88 SJR 0.559 SNIP 0.748
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.79 SJR 0.495 SNIP 0.603
Metal alloys for the new generation of compressors at hydrogen stations: Parametric study of corrosion behavior

Compressors are one of the most costly components at hydrogen stations, which leads to the high price of hydrogen production. The substitution of a solid piston with ionic liquid is a promising option that may solve some of the challenges related to conventional reciprocating compressors and, consequently, significantly reduce the final cost of hydrogen production. The correct choice of ionic liquid and construction materials is critical for avoiding significant corrosion problems. Hence, the objective of this study is to evaluate the compatibility of various austenitic stainless steels and nickel-based alloys as construction materials in contact with 80 °C ionic liquids in an ionic liquid hydrogen compressor, considering the role of parameters such as the temperature, viscosity, ionic liquid cation and anion, and water absorption. The results show that temperature contributes to increasing the corrosion rate. However, even at 80 °C, the very low corrosion current densities proved that all of the tested alloys are safe to use as construction materials. AISI 347 showed very high corrosion resistance in all of the ionic liquids. The highest corrosion resistance among all of the tested alloys was observed in trihexyltetradecylphosphonium bis (trifluoromethylsulfonyl) imide, which had a relatively high viscosity and the lowest water content.
Metal–organic frameworks-derived honeycomb-like Co$_3$O$_4$/three-dimensional graphene networks/Ni foam hybrid as a binder-free electrode for supercapacitors

The honeycomb-like porous Co$_3$O$_4$ grown on three dimensional graphene networks/nickel foam (3DGN/NF) has been successfully prepared by a facile solution growth process with subsequent annealing treatment, in which the Co-based metal organic framework (ZIF-67) act as the precursor of the metal oxide. The Co$_3$O$_4$/three-dimensional graphene networks/Ni foam (Co$_3$O$_4$/3DGN/NF) hybrid as the electrode for supercapacitor can deliver high specific capacitance (321 F g$^{-1}$ at 1 A g$^{-1}$) and excellent long-cycling stability (88% of the maximum capacitance after 2000 charge-discharge cycles). Furthermore, the Co$_3$O$_4$/3DGN/NF hybrid exhibits the maximum energy density of 7.5 W h kg$^{-1}$ with the power density of 794 W kg$^{-1}$ and remain 4.1 W h kg$^{-1}$ with the power density of 15 kW kg$^{-1}$ in the two-electrode system. The enhanced electrochemical properties can be attributed to the unique nanostructure of Co$_3$O$_4$ with admirable pseudocapacitance performance and the intimate integration of graphene with the Co$_3$O$_4$ and the Ni foam matrix, which not only enhances the electron conductivity for fast electron and ion transport but also provides high specific surface area and excellent structural stability.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors, Tianjin University
Authors: Deng, X. (Ekstern), Li, J. (Ekstern), Zhu, S. (Ekstern), He, F. (Ekstern), He, C. (Ekstern), Liu, E. (Ekstern), Shi, C. (Ekstern), Li, Q. (Intern), Zhao, N. (Ekstern)
Number of pages: 9
Pages: 16-24
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Alloys and Compounds
Volume: 693
ISSN (Print): 0925-8388
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SJR 1.02 SNIP 1.403 CiteScore 3.66
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.05 SJR 0.954 SNIP 1.332
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.957 SNIP 1.398 CiteScore 3.03
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.117 SNIP 1.632 CiteScore 3.13
Web of Science (2014): Indexed yes
Micromechanics Models for Viscoelastic Plain-Weave Composite Tape Springs

The viscoelastic behavior of polymer composites decreases the deployment force and the postdeployment shape accuracy of composite deployable space structures. This paper presents a viscoelastic model for single-ply cylindrical shells (tape springs) that are deployed after being held folded for a given period of time. The model is derived from a representative unit cell of the composite material, based on the microstructure geometry. Key ingredients are the fiber volume density in the composite tows and the constitutive behavior of the fibers (assumed to be linear elastic and transversely isotropic) and of the matrix (assumed to be linear viscoelastic). Finite-element-based homogenizations at two scales are conducted to obtain the Prony series that characterize the orthotropic behavior of the composite tow, using the measured relaxation modulus of the matrix as an input. A further homogenization leads to the lamina relaxation ABD matrix. The accuracy of the proposed model is verified against the experimentally measured time-dependent compliance of single lamina in either pure tension or pure bending. Finite element simulations of single-ply tape springs based on the proposed model are compared to experimental measurements that were also obtained during this study.

General information
Microscopic origin of the mobility enhancement at a spinel/perovskite oxide heterointerface revealed by photoemission spectroscopy

The spinel/perovskite heterointerface γ-Al2O3/SrTiO3 hosts a two-dimensional electron system (2DES) with electron mobilities exceeding those in its all-perovskite counterpart LaAlO3/SrTiO3 by more than an order of magnitude, despite the abundance of oxygen vacancies which act as electron donors as well as scattering sites. By means of resonant soft x-ray photoemission spectroscopy and \textit{ab initio} calculations, we reveal the presence of a sharply localized type of oxygen vacancies at the very interface due to the local breaking of the perovskite symmetry. We explain the extraordinarily high mobilities by reduced scattering resulting from the preferential formation of interfacial oxygen vacancies and spatial separation of the resulting 2DES in deeper SrTiO3 layers. Our findings comply with transport studies and pave the way towards defect engineering at interfaces of oxides with different crystal structures.
Microstructural and electrical characterization of Mn-Co spinel protective coatings for solid oxide cell interconnects

Electrophoretic deposition, thermal co-evaporation and RF magnetron sputtering methods are used for the preparation of Mn-Co based ceramic coatings for solid oxide fuel cell steel interconnects. Both thin and relatively thick coatings (1–15 μm) are prepared and characterised for their potential protective behaviour. Mn-Co coated Crofer22APU samples are electrically tested for 5000 h at 800 °C under a 500 mA cm⁻² current load to determine their Area Specific Resistance increase due to a growing chromia scale. After tests, samples are analysed by scanning and transmission electron microscopy. Analysis is focused on the potential chromium diffusion to or through the coating, the oxide scale thickness and possible reactions at the interfaces. The relationships between the coating type, thickness and effectiveness are reviewed and discussed. Out of the three Mn-Co coatings compared in this study, the one deposited by electrophoretic deposition presents the best protection against Cr diffusion and offers long term stability.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Politecnico di Torino, Edison Research & Development Center, AGH University of Science and Technology, University of Erlangen-Nuremberg
Authors: Molin, S. (Intern), Sabato, A. G. (Ekstern), Bindi, M. (Ekstern), Leone, P. (Ekstern), Cempura, G. (Ekstern), Salvo, M. (Ekstern), Cabanas Polo, S. (Ekstern), Boccaccini, A. R. (Ekstern), Smeacetto, F. (Ekstern)
Pages: 4781-4791
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of the European Ceramic Society
Volume: 37
Issue number: 15
ISSN (Print): 0955-2219
Ratings:
BFI (2018): BFI-level 1
Solid oxide cell, Electrophoretic deposition, Protective coating, Area specific resistance, Microstructure

DOIs:
Source: FindIt
Source-ID: 2373095017
Publication: Research - peer-review › Journal article – Annual report year: 2017
Microstructural Characterization of Ni/YSZ Electrodes in a Solid Oxide Electrolysis Stack Tested for 9000 Hours

The effects of long-term operation in electrolysis mode on the microstructure of Ni/YSZ electrodes were investigated. The electrode structures were investigated in “as reduced” state and after 9000 h of operation in a 25 cell stack. Microstructural data were obtained by scanning electron microscopy and focused-ion-beam serial sectioning. Microstructural characteristics were extracted by 1D and 3D methods. Significant microstructural changes were observed between the two cells analyzed. A significant loss of Ni in the active electrode is observed, from ~ 29% (by volume) in the reference cell to ~ 24% as well as a coarsening of the Ni particle sizes. The long-term tested cell shows lower percolating triple phase boundary density (0.76 µm/µm³) than the un-tested reference (2.0 µm/µm³). This reduction is mainly due to the loss of triple phase boundary percolation through the Ni phase where a reduction from a percolation degree above 90% to ~50% is observed.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Imaging and Structural Analysis, Applied Electrochemistry
Authors: Trini, M. (Intern), Jørgensen, P. S. (Intern), Hauch, A. (Intern), Chen, M. (Intern), Hendriksen, P. V. (Intern)
Pages: 3049-3064
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: E C S Transactions
Volume: 78
Issue number: 1
ISSN (Print): 1938-5862
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 0.44 SJR 0.225 SNIP 0.252
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 0.4 SJR 0.228 SNIP 0.253
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.211 SNIP 0.244 CiteScore 0.36
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.212 SNIP 0.234 CiteScore 0.36
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.192 SNIP 0.231 CiteScore 0.27
ISI indexed (2013): ISI indexed no
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.241 SNIP 0.26 CiteScore 0.29
ISI indexed (2012): ISI indexed no
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.261 SNIP 0.28 CiteScore 0.36
ISI indexed (2011): ISI indexed no
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.249 SNIP 0.251
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.242 SNIP 0.27
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.254 SNIP 0.255
Scopus rating (2007): SJR 0.213 SNIP 0.206
Scopus rating (2006): SJR 0.134 SNIP 0.073
Original language: English
Electronic versions:
ECSTransaction_martina_trini_post_print_from_DTU_Energy.pdf
DOIs:
10.1149/07801.3049ecst
Microstructural Characterization of Ni/YSZ Electrodes in a Solid Oxide Electrolysis Stack Tested for 9000 Hours

**General information**
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Imaging and Structural Analysis, Applied Electrochemistry
Authors: Trini, M. (Intern), Jørgensen, P. S. (Intern), Hauch, A. (Intern), Chen, M. (Intern), Hendriksen, P. V. (Intern)
Number of pages: 1
Publication date: 2017

**Host publication information**
Title of host publication: ECS Meeting Abstracts
Volume: MA2017-03
Publisher: The Electrochemical Society
Article number: 201
Main Research Area: Technical/natural sciences
Conference: 15th International Symposium on Solid Oxide Fuel Cells (SOFC-XV), Hollywood, United States, 23/07/2017 - 23/07/2017
Links:
http://ma.ecsdl.org.proxy.findit.dtu.dk/content/MA2017-03/1/201

Microstructure and chemical data of the thermoelectric ZnSb material after joining to metallic electrodes and heat treatment
The data presented in this article are related to the research article entitled: “Solder free joining as a highly effective method for making contact between thermoelectric materials and metallic electrodes” (Malik et al., 2017) [1]. This article presents microstructure obtained by scanning electron microscopy (SEM) and chemical analysis by energy dispersive X-ray spectroscopy (EDX) point measurements of the thermoelectric ZnSb legs after joining to metallic electrodes using solder (Zn-2Al) and free-soldering methods.

**General information**
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Electrofunctional materials
Authors: Malik, S. A. (Intern), Le, T. H. (Intern), Van Nong, N. (Intern)
Pages: 97-101
Publication date: 2017
Main Research Area: Technical/natural sciences

**Publication information**
Journal: Data in Brief
Volume: 15
ISSN (Print): 2352-3409
Ratings:
Scopus rating (2017): CiteScore 0.7
Scopus rating (2016): CiteScore 0.5
Scopus rating (2015): CiteScore 0.25
Original language: English
Electronic versions:
1_s2.0_S2352340917304547_main.pdf
1_s2.0_S2352340917304547_main.pdf
DOIs:
10.1016/j.dib.2017.09.023
Source: PublicationPreSubmission
Source-ID: 137100446
Publication: Research - peer-review » Conference abstract in proceedings – Annual report year: 2017

Microstructure and Electrical Properties of Fe,Cu Substituted (Co,Mn)₃O₄ Thin Films
In this work, thin films (~1000 nm) of a pure MnCo₂O₄ spinel together with its partially substituted derivatives (MnCo₁₂₆Cu₀₂Fe₀₂O₄, MnCo₁₂₆Cu₀₄O₄, MnCo₁₂₆Fe₀₂O₄) were prepared by spray pyrolysis and were evaluated for electrical conductivity. Doping by Cu increases the electrical conductivity, whereas doping by Fe decreases the conductivity. For Cu
containing samples, rapid grain growth occurs and these samples develop cracks due to a potentially too high thermal expansion coefficient mismatch to the support. Samples doped with both Cu and Fe show high electrical conductivity, normal grain growth and no cracks. By co-doping the Mn, Co spinel with both Cu and Fe, its properties can be tailored to reach a desired thermal expansion coefficient/electrical conductivity value.

**General information**

State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Gdansk University of Technology
Authors: Szymczewska, D. (Ekstern), Molin, S. (Intern), Hendriksen, P. V. (Intern), Jasinski, P. (Ekstern)
Number of pages: 12
Publication date: 2017
Main Research Area: Technical/natural sciences

**Publication information**

Journal: Crystals
Volume: 7
Issue number: 7
Article number: 185
ISSN (Print): 2073-4352
Ratings:
Web of Science (2018): Indexed yes
Scopus rating (2017): CiteScore 1.97 SJR 0.566 SNIP 0.745
Web of Science (2017): Indexed Yes
Scopus rating (2016): CiteScore 1.89 SJR 0.544 SNIP 0.768
Web of Science (2016): Indexed yes
Scopus rating (2015): SJR 0.567 SNIP 0.713 CiteScore 1.47
Scopus rating (2014): SJR 0.464 SNIP 0.648 CiteScore 1.03
Web of Science (2014): Indexed yes
Scopus rating (2013): SJR 0.355 SNIP 0.684 CiteScore 0.77
ISI indexed (2013): ISI indexed no
Scopus rating (2012): SJR 0.182 SNIP 0.257
ISI indexed (2012): ISI indexed no
Original language: English
Manganese cobalt spinel, High temperature protective coatings, Thin films, Electrical conductivity

Electronic versions:
crystals_07_00185_v2.pdf
DOIs:
10.3390/cryst7070185
Source: FindIt
Source-ID: 2372198173
Publication: Research - peer-review › Journal article – Annual report year: 2017

**Mid-IR optical properties of silicon doped InP**

InP is one of the most important materials for optoelectronics as a direct bandgap semiconductor, which can also be regarded as a low loss alternative plasmonic material for mid-infrared (mid-IR). The InP films studied in this work were grown by metal-organic vapor phase epitaxy (MOVPE). The effect of growth conditions on the optical and electrical properties of silicon doped InP (InP:Si) in the wavelength range from 3 to 40 μm was studied. The carrier concentration of up to 3.9 × 10¹⁹ cm⁻³ is achieved by optimizing the growth conditions. The dielectric function, effective mass of electrons and plasma frequency were determined by Fourier transform infrared spectroscopy (FTIR) for different carrier density levels. The plasma frequency can be tuned effectively via doping from 18.43 to 50.5 THz. Based on the experimental results, a semi-empirical formula for the plasma frequency, as a function of carrier concentration, is derived. Comparison to other semiconductors shows superior plasmonic performance of InP:Si in terms of propagation length and surface confinement.

**General information**

State: Published
Organisations: Plasmonics and Metamaterials, Department of Energy Conversion and Storage, Mixed Conductors, Electrofunctional materials, Department of Photonics Engineering, Nanophotonic Devices, St. Petersburg Academic University
Authors: Panah, M. E. A. (Intern), Han, L. (Intern), Normant, K. (Intern), Pryds, N. (Intern), Nadtochiy, A. (Ekstern), Zhukov, A. E. (Ekstern), Lavrinenko, A. (Intern), Semenova, E. (Intern)
Pages: 2260-2271
Model for solid oxide fuel cell cathodes prepared by infiltration

A 1-dimensional model of a cathode has been developed in order to understand and predict the performance of cathodes prepared by infiltration of La0.6Sr0.4Co1.05O3-δ (LSC) into porous backbones of Ce0.9Gd0.1O1.95 (CGO). The model accounts for the mixed ionic and electronic conductivity of LSC, ionic conductivity of CGO, gas transport in the porous cathode, and the oxygen reduction reaction at the surface of percolated LSC. Geometrical variations are applied to reflect a changing microstructure of LSC under varying firing temperatures. Using microstructural parameters obtained from detailed scanning electron microscopy and simulations of the measured polarization resistances, an expression for the area specific resistance (rp) associated with the oxygen exchange on the surface of the infiltrated LSC particles was extracted and compared with literature values. A series of microstructural parameter variations are presented and discussed with the aim of presenting specific guidelines for optimizing the microstructure of cathodes prepared by infiltration.

General information

State: Published
Organisations: Mixed Conductors, Department of Energy Conversion and Storage
Authors: Samson, A. J. (Intern), Søgaard, M. (Intern), Hendriksen, P. V. (Intern)
Pages: 73-95
Publication date: 2017
Main Research Area: Technical/natural sciences
Modeling a material from packing, through sintering and to the final microstructural properties

We present a combination of numerical models that can together simulate the initial packing of particles, followed by sintering and finally the resulting microstructural properties. For the latter we here focus on the magnetism of a sintered sample, and the associated coupling between heat and magnetism known as the magnetocaloric effect. We present a 3-dimensional time-dependent numerical model that spatially resolves samples down to the grain size, and includes the demagnetizing field, chemical inhomogeneity realized as a spatial variation of Curie temperature across the sample, local hysteresis and heat transfer. We can thus model how particle size, packing, sintering and chemical inhomogeneity affect the observed properties of magnetocaloric samples. For example, we show that even a modest distribution in Curie temperature (TC) across the sample results in a significant broadening and lowering of the total entropy change of the sample around TC. We discuss how clustering of grains with similar values of TC across the sample influences the results.

Modeling of Ni Diffusion Induced Austenite Formation in Ferritic Stainless Steel Interconnects

Ferritic stainless steel interconnect plates are widely used in planar solid oxide fuel cell and electrolysis cell stacks. During stack production and operation, nickel from the Ni/yttria stabilized zirconia fuel electrode or from the Ni contact component layer diffuses into the interconnect plate, causing transformation of the ferritic phase into an austenitic phase in the interface region. This is accompanied with changes in volume, and in mechanical and corrosion properties of the interconnect plates. In this work, kinetic modeling of the inter-diffusion between Ni and FeCr based ferritic stainless steel was conducted, using the CALPHAD (CALculation of PHAse Diagrams) approach with the DICTRA (Diffusion Controlled TRAnsformation) software. The kinetics of inter-diffusion and austenite formation was explored in detail. The simulation was further validated by comparing with experiments. The results show that after 2000 h at 800°C Ni diffuses more than 100 μm deep into Crofer 22 APU. Along with the Ni diffusion, part of the ferritic steel with 50–60 μm in thickness has transformed into the austenitic phase. Growth of the austenite phase in commercial interconnect materials was predicted to take place under practical stack operation conditions.
Model of Organic Solar Cell Photocurrent Including the Effect of Charge Accumulation at Interfaces and Non-Uniform Carrier Generation
We developed an improved model to fit the photocurrent density versus voltage in organic solar cells. The model has been validated by fitting data from P3HT:PCBM solar cells. Our model quantitatively accounts for the band bending near the electrodes caused by charge accumulation in the active layer. The model explains the position of the built-in and the zero-field voltage, the value of the internal electric field, the impact of electrode materials, and the appearance of multiple inflections. In addition, the model can be used to monitor the cell condition during accelerated lifetests.

**General information**

State: Published
Organisations: Department of Energy Conversion and Storage, Organic Energy Materials, University of Padua
Authors: Torto, L. (Ekstern), Cester, A. (Ekstern), Rizzo, A. (Ekstern), Wrachien, N. (Ekstern), Gevorgyan, S. (Intern), Corazza, M. (Intern), Krebs, F. C. (Intern)
Pages: 387-395
Publication date: 2017
Main Research Area: Technical/natural sciences

**Publication information**

Volume: 4
Issue number: 6
ISSN (Print): 2168-6734
Ratings:
Web of Science (2018): Indexed yes
Scopus rating (2017): CiteScore 3.37 SJR 1.016 SNIP 1.436
Web of Science (2017): Indexed yes
Scopus rating (2016): CiteScore 3.47 SJR 1.179 SNIP 2.136
Scopus rating (2015): SJR 0.965 SNIP 2.28 CiteScore 2.67
Scopus rating (2014): SJR 0.662 SNIP 1.756
Original language: English
Organic solar cells, Analytical model
Electronic versions:
J_EDS_Final_Paper_Main_document_PDF.pdf
07549082.pdf
DOIs:
10.1109/JEDS.2016.2602563
Publication: Research - peer-review › Journal article – Annual report year: 2017

Molecular dynamics simulation of radiation grafted FEP films as proton exchange membranes: Effects of the side chain length

In order to study the microstructure of the prepared potential proton exchange membrane (PEM), molecular dynamics (MD) simulations were used to elucidate the transport behavior of water molecules and hydronium ions inside the hydrated sulfonated styrene grafted fluorinated ethylene propylene (FEP) membrane, which possess different side chain lengths. By evaluating the radial distribution functions (RDFs), it was observed that with increasing side chain length, the average sulfur-hydronium ion separation slightly increased and the coordination number of H3O+ around sulfonic acid groups decreased whereas larger water clusters formed. The results of the mean square displacements (MSDs) show that the proton conductivities of the membranes with the proposed side chain lengths were about three fifths of the experimental data, of which the membrane with side chain length of 7 sulfoionic styrene units was supposed to exhibit the highest proton conductivity, that is 115.69 mS cm⁻¹. All of the supposed membrane models presented good proton conductivity that could definitely meet the application requirements of the proton exchange membranes. The MD simulations can provide an insight to the chain structure of the radiation grafted membrane, and are of guidance significance to design other side-chain-structure polymers to be used as PEMs in proton exchange membrane fuel cells (PEMFCs).

**General information**

State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors, Tsinghua University
Authors: Li, X. (Ekstern), Zhao, Y. (Ekstern), Li, W. (Ekstern), Wang, S. (Ekstern), Liu, X. (Ekstern), Xie, X. (Ekstern), Chen, J. (Ekstern), Li, Q. (Intern), Jensen, J. O. (Intern)
Pages: 29977-29987
Publication date: 2017
Main Research Area: Technical/natural sciences

**Publication information**

Volume: 42
Fused-pentagons results in an increase of local steric strain according to the isolated pentagon rule (IPR), and for all reported non-IPR clusterfullerenes multiple (two or three) metals are required to stabilize the strained fused-pentagons, making it difficult to access the single-atom properties. Herein, we report the syntheses and isolations of novel non-IPR mononuclear clusterfullerenes MNC@C76 (M=Tb, Y), in which one pair of strained fused-pentagon is stabilized by a mononuclear cluster. The molecular structures of MNC@C76 (M=Tb, Y) were determined unambiguously by single-crystal X-ray diffraction, featuring a non-IPR C2v(19138)-C76 cage entrapping a nearly linear MNC cluster, which is remarkably different from the triangular MNC cluster within the reported analogous clusterfullerenes based on IPR-obeying C82 cages. The TbNC@C76 molecule is found to be a field-induced singlemolecule magnet (SMM).
Multiphase oxygen electrodes for solid oxide electrolysis cells

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors
Authors: Tripkovic, D. (Intern), Hendriksen, P. V. (Intern), Mogensen, M. B. (Intern)
Publication date: 2017
Event: Abstract from 21st International Conference on Solid State Ionics, Padova, Italy.
Main Research Area: Technical/natural sciences
Electronic versions:
SS121_abstract_DJTRI.pdf

Relations
Activities:
Multiphase oxygen electrodes for solid oxide electrolysis cells
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2017

Nanostructured Materials: Enhancing the Thermoelectric Performance
Near-net shape manufacture of $\text{B}_4\text{C}$–Co and $\text{ZrC}$–Co composites by slip casting and pressureless sintering

Fabrication of near-net shaped $\text{B}_4\text{C}$–Co and $\text{ZrC}$–Co composites by slip casting and pressureless sintering is described. It is shown how $\text{B}_4\text{C}$–Co and $\text{ZrC}$–Co concentrated suspensions can be prepared by aqueous colloidal processing, and optimized (in terms of pH, deflocculant contents, and sonication time) to have a shear-thinning rheological behaviour suitable for the near-net shaping of the corresponding cermet compacts by slip casting. It is also demonstrated that the robust, highly-dense compacts so obtained have a uniform green microstructure without macro-defects or gradient density, and which can be fully densified by pressureless sintering. Specifically, it is shown that $\text{B}_4\text{C}$–Co compacts densify by reactive and transient liquid-phase sintering, thus resulting in multi-component ceramics. $\text{ZrC}$–Co compacts densify however by persistent liquid-phase sintering, thus resulting in cermets. An explanation is given for these observations, and general implications are discussed for the near-net shape manufacture of these and similar carbide-metal composites for use in engineering applications.
New Light Source Setup for Angle Resolved Light Absorption measurement of PV sample

Here, we introduce measurements of angle resolved light absorption by PV cells, using broadband laser driven white light source with a bright, stable, broad spectral range and well collimated light.

General information
State: Published
Number of pages: 1
Publication date: 2017
Main Research Area: Technical/natural sciences
Absorption, Collimated, Reproducibility, Laser
Electronic versions:
Amdemeskel_Abstract_.pdf

Relations
Projects:
New Light Source Setup for Angle Resolved Light Absorption measurement of PV sample
Novel materials for more robust solid oxide fuel cells in small scale applications

Solid oxide fuel cells can offer supply of electrical energy with a high efficiency and based on a wide range of fuels. While natural gas and/or bio methane is a commonly used fuel for combined heat and power supply, liquid fuels such as gasoline, Diesel and alcohols are interesting fuels, especially for remote fuel cell systems. For those applications, redox tolerant and Sulphur resistant fuel electrode materials are advantageous in order to make the cells more tolerant against sudden system failures such as fuel cut off and reformer breakdown. Also for direct feeding of alcohols and higher hydrocarbons, coking tolerant electrodes are required. State-of art fuel electrodes are based on a nickel ceramic composite, a nickel cermet, which suffers from low redox stability, susceptibility for sulfur poisoning and coking. Redox stable anodes can be achieved by replacing the Ni-cermet fuel electrode by an electronically conducting ceramic, e.g. strontium titanate with incorporated nano-scaled electro catalysts. Full cells using LSM/YSZ cathodes have been developed and tested as single 5 x 5 cm2 cells and up 100 cm2 circular cells. The initial performance exceeded 0.4 W/cm2 at 850 °C and redox tolerance has been proven in a 1 kW system environment. The cell concept provides flexibility with respect to the used electro-catalysts and various metals including Ni and Ru infiltrated in a niobium modified strontium titanate have been studied as regards their electrochemical performance and stability. Stable power output has been observed for Ru and Ru/Gd modified ceria (CGO) as infiltrate. The stability of the nano scaled electro catalysts depends on the materials combinations and the role of the possible catalyst-support interactions will be discussed.

NOx Selective Catalytic Reduction (SCR) on Self-Supported V-W-doped TiO2 Nanofibers

Electrospun V–W–TiO2 catalysts, resulting in a solid solution of V and W in the anatase phase, are prepared as nonwoven nanofibers for NOx selective catalytic reduction (SCR). Preliminary catalytic characterization indicates their superior NOx conversion efficiency to the-state-of-the-art material. A novel concept of a self-supported, ultra-compact, and lightweight nanofibrous SCR-reactor is defined.

General information

State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Fundamental Electrochemistry, Mixed Conductors, Technical University of Denmark
Pages: 3466-3472
Publication date: 2017
Main Research Area: Technical/natural sciences
Nucleophilic stabilization of water-based reactive ink for titania-based thin film inkjet printing

Drop on demand deposition (DoD) of titanium oxide thin films (<500 nm) is performed via a novel titanium-alkoxide-based solution that is tailored as a reactive ink for inkjet printing. The ink is developed as water-based solution by a combined use of titanium isopropoxide and n-methyldiethanolamine (MDEA) used as nucleophilic ligand. The function of the ligand is to control the fast hydrolysis/condensation reactions in water for the metal alkoxide before deposition, leading to formation of the TiO$_2$ only after the jet process. The evolution of the titanium-ligand interactions at increasing amount of MDEA is here elucidated in terms of long term stability. The ink printability parameter ($Z$) is optimized, resulting in a reactive solution with printability, $Z$, >1, and chemical stability up to 600 h. Thin titanium oxide films (<500 nm) are proved on different substrates. Pure anatase phase is obtained after annealing at low temperature (ca. 400 °C).
Numerical routine for magnetic heat pump cascading

Heat pumps use low-temperature heat absorbed from the energy source to create temperature gradient (TG) across the energy sink. Magnetic heat pumps (MHP) can perform this function through operating active magnetic regeneration (AMR) cycle. For building heating, TGs of up to a few K might be necessary, which is hardly achievable with a single MHP and such techniques as cascading are required. Series and parallel cascading increase the AMR span and heating power, respectively, but do not change TG. Therefore, the intermediate type of cascading was proposed with individual MHPs separately connected at their cold and hot sides [1].

In these works, a single MHP is separated into smaller cascaded MHPs with the same total mass. This kind of mass redistribution is hard to implement experimentally since several prototypes with different AMR number and sizes should be constructed. In this theoretical study, instead of changing individual AMR sizes, we rearranged parallel-connected AMRs in separate blocks (HP1, HP2 and HP3 in Fig. 1(a)) and connected the cold (hot) outlet of one block to the cold (hot) inlet of the next block giving a cascading configuration. Thus, not only the total mass but also the total number of AMRs remain constant, making this configuration easier to implement.

A MATLAB routine for cascading simulation from a single AMR data was implemented. Calculated heating power for configuration in Fig. 1(a) is plotted in Fig. 1(b) and the cold- and hot-side TGs are around 2 K and 3 K. Changing the number of MHPs, we optimized input parameters to achieve maximum heating powers. We have found that both maximum heating power and COP decrease together with number of heat pumps, but the TGs and the temperature span can be largely increased. References [1] M. Tahavori et al., "A Cascading Model Of An Active Magnetic Regenerator System", In Proceedings of the 7th International Conference on Magnetic Refrigeration at Room Temperature (2016) 248-251

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, University of Southern Denmark
Authors: Filonenko, K. (Ekstern), Lei, T. (Intern), Engelbrecht, K. (Intern), Bahl, C. (Intern), Veje, C. (Ekstern)
Number of pages: 1
Publication date: 2017
Event: Poster session presented at Danish Days 2017 on Caloric Materials and Devices, Roskilde, Denmark.
Main Research Area: Technical/natural sciences
Electronic versions:
numerical.pdf
Source: FindIt
Source-ID: 2391784725
Publication: Research - peer-review › Poster – Annual report year: 2017

On the Properties and Long-Term Stability of Infiltrated Lanthanum Cobalt Nickelates (LCN) in Solid Oxide Fuel Cell Cathodes

Infiltration as a fabrication method for solid oxide fuel cells (SOFC) electrodes is offering significant improvements in cell performance at reduced materials and fabrication costs, especially when combined with co-sintering. However, important questions regarding the long-term performance and microstructural stability remain unanswered. Here, we present the results of a three-year project, where large footprint anode-supported SOFCs with a co-sintered cathode backbone and infiltrated La0.95Co0.4Ni0.6O3 (LCN) cathodes were developed and thoroughly characterized. The initial long-term performance and stability of this new cell type was investigated for 1500+ hours, coupled with STEM-EDS investigation of the microstructural changes in the infiltrated electrodes. Additionally, electrodes were further aged at elevated temperatures (750 - 900°C) for periods reaching up to 5000 hours, while following changes in the electrode properties using SEM, BET area, and in-plane conductivity measurements. Finally, the mechanical properties of co-sintered cathode backbone cells were determined in four-point bending tests carried out both at room temperature and at 800°C in air. Based on these results, degradation mechanisms were identified and recommendation for safe operation conditions in real life application could be formulated.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Fundamental Electrochemistry, Imaging and Structural Analysis, Haldor Topsoe AS
Pages: F748-F758
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of the Electrochemical Society
Volume: 164
Issue number: 7
On the way towards smart energy supply in cities: The impact of interconnecting geographically distributed district heating grids on the energy system

A linear continuous optimization model with an hourly time resolution was developed in order to model the impact of subsequent interconnections of different DH grids. The municipality of Sønderborg was chosen for a case study and interconnections of five currently disconnected DH grids were assessed. Moreover, the impact of industrial waste heat on the DH supply was also assessed. In the reference year (2013) two out of four interconnections proved to be economically viable. The results for the future energy system (2029) showed that interconnecting geographically distributed DH grids reduces primary energy supply by 9.5%, CO₂ emissions by 11.1% and total system costs by 6.3%. Inclusion of industrial waste heat in the fully interconnected DH grid reduced primary energy supply for an additional 3%, CO₂ emissions for an additional 2.2% and total system costs for an additional 1.3%. The case of the future energy supply system with interconnected DH grids and installed industrial waste heat recuperation results in the lowest primary energy demand, emissions and costs. Finally, the benefits of the interconnected DH grid, in terms of system flexibility, CO₂ emissions, total costs and energy efficiency, proved to be much greater in the future energy system.
Operational test of bonded magnetocaloric plates

Bonded plates made by hot pressing La\textsubscript{0.85}Ce\textsubscript{0.15}Fe\textsubscript{11.25}Mn\textsubscript{0.25}Si\textsubscript{1.5}H\textsubscript{2} particles and resin have been tested as active magnetic regenerators in a small scale magnetocaloric device. Firstly the plates were carefully characterised magnetically and thermally. The plates were prepared with 5 wt% resin, and from density measurements it was found that the volume ratio of the magnetocaloric material in the plates was 0.53, due to the resin and porosity. The best operating conditions for the plate regenerator were determined at which a temperature span of 6.4 K was measured along the plates.

General information

State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Chinese Academy of Sciences, University of Science and Technology Beijing
Pages: 245-251
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information

Journal: International Journal of Refrigeration
Volume: 76
ISSN (Print): 0140-7007
Ratings:
BFI (2018): BFI-level 1
Biomass is one renewable energy source, which is independent from solar radiation and wind effect. Solid oxide fuel cells (SOFC’s) are able to convert landfill gas derived from landfill directly into electricity and heat with a high efficiency. In the present work a planar 16cm² SOFC cell was operated with a real landfill gas from one of the largest Danish waste dump sites and additional carbon dioxide reforming agent at 750°C, both with gas cleaning through an active carbon filter and...
The tests showed an electric efficiency up to ~60%. It was found that the active carbon filter was necessary to prevent poisoning and thereby to decrease the degradation rate.

**General information**

State: Published
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry
Authors: Langnickel, H. (Intern), Hagen, A. (Intern)
Pages: 417-418
Publication date: 2017

**Host publication information**

Title of host publication: Proceedings of the 7th European Fuel Cell Technology & Applications Conference (EFC2017)
Publisher: ENEA
Editor: Cigolotti, V.
Article number: EFC17257
ISBN (Print): 978-88-8286-324-1
Main Research Area: Technical/natural sciences
Conference: 7th European Fuel Cell Technology & Applications Conference (EFC2017), Naples, Italy, 12/12/2017 - 12/12/2017
Landfill gas, Solid oxide fuel cell, Efficiency, Dry reforming, Poisoning

**Electronic versions:**

EFC17257_Revised.pdf

**Links:**

http://www.europeanfuelcell.it/images/proceedings_EFC17.pdf

Source: PublicationPreSubmission
Source-ID: 142167177
Publication: Research - peer-review › Article in proceedings – Annual report year: 2017

**Orientation-Dependent Oxygen Evolution on RuO₂ without Lattice Exchange**

RuO₂ catalysts exhibit record activities toward the oxygen evolution reaction (OER), which is crucial to enable efficient and sustainable energy storage. Here we examine the RuO₂ OER kinetics on rutile (110), (100), (101), and (111) orientations, finding (100) the most active. We assess the potential involvement of lattice oxygen in the OER mechanism with online electrochemical mass spectrometry, which showed no evidence of oxygen exchange on these oriented facets in acidic or basic electrolytes. Similar results were obtained for polyoriented RuO₂ films and particles, in contrast to previous work, suggesting lattice oxygen is not exchanged in catalyzing OER on crystalline RuO₂ surfaces. This hypothesis is supported by the correlation of activity with the number of active Ru-sites calculated by density functional theory, where more active facets bind oxygen more weakly. This new understanding of the active sites provides a design strategy to enhance the OER activity of RuO₂ nanoparticles by facet engineering.

**General information**

State: Published
Organisations: Department of Physics, Department of Energy Conversion and Storage, Atomic scale modelling and materials, Massachusetts Institute of Technology, Leiden University, Oak Ridge National Laboratory, University of Copenhagen
Pages: 876-881
Publication date: 2017
Main Research Area: Technical/natural sciences

**Publication information**

Journal: ACS Energy Letters
Volume: 2
Issue number: 4
Ratings:

BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 10.24
Original language: English

**Electronic versions:**

RuO₂_OLEMS_vR.pdf. Embargo ended: 16/03/2018

DOIs:

10.1021/acsenergylett.7b00135
Overcoming the Scaling Lag for Polymer Solar Cells

There is a long stretch between a laboratory discovery and a practical demonstration. For a potentially useful energy technology, many further strides must be taken before a societally meaningful scale is reached. In this work we have, based on many past experiences, brought the fully roll-to-roll printed polymer solar cell to a realistic scale across the entire value chain. The materials synthesis, the manufacture, the installation, the failure modes, and the operation have all been covered and addressed. We demonstrate outdoor operation for 2 years through a large-scale, grid-tied, high-voltage system and show that thin plastic foil can be operated as an energy-producing technology. Critical to the demonstration was the identification of the drying method during printing, and we show how this development relates to the scaling lag (the period between the point in time for a laboratory demonstration and the point in time for scaled manufacture) and allows for closure of the scaling gap.

Oxygen Permeation and Stability Study of (La0.6Ca0.4)0.98(Co0.8Fe0.2)O3-δ Membranes: Alternative title; Oxygen permeation and stability study of (La0.6Ca0.4)(0.98)(Co0.8Fe0.2)O3-delta membranes

The perovskite-type oxide (La0.6Ca0.4)0.98(Co0.8Fe0.2)O3-δ (LCCF) was investigated for use as oxygen separation membrane. A 25 µm thick dense membrane on a porous LCCF support with a thickness of around 175 µm was prepared by a tape casting and lamination process. The optimum sintering temperature of the component was established to be 1050 °C by analysis of microstructures of membranes sintered at different temperatures. Scanning electron microscopy (SEM) examination of cross-sections of the sintered membrane showed that it consisted of two phases, the main phase being enriched in calcium (Ca) and depleted in lanthanum (La), relative to the nominal composition. A surface activation layer of LCCF was deposited onto the dense layer to increase the exchange rate of oxygen at the surface. For the coated membrane, the oxygen permeation flux increased with temperature and reached a maximum value of 3.32 Nml cm−2 min−1 at 900 °C when, for characterization purpose pure oxygen was used as feed and a maximum value of 2.06 Nml cm−2 min−1 at 900 °C was obtained when air was used at the feed side, both with N2 sweep on the permeate side. The stability of the membrane against sulfur dioxide (SO2) and pure carbon dioxide (CO2) was tested. A small decrease in the flux was observed over 48 h in CO2 at 850 °C. SEM examinations of the cross-section of the tested membrane showed that the Ca rich phase in the membrane showed a tendency to migrate to the feed side. Whereas the material shows a CO2 stability superior to that of Sr or Ba containing analogues, the material stability is not sufficient for applications requiring direct exposure to sulfur-rich flue gases.
Oxygen permeation membrane, Kinetic demixing, Stability, Oxy-fuel
DOI: 10.1016/j.memsci.2017.07.050
Source: PublicationPreSubmission
Source-ID: 134380925
Publication: Research - peer-review › Journal article – Annual report year: 2017

Oxygen transport properties of tubular Ce$_{0.9}$Gd$_{0.1}$O$_{1.95}$-La$_{0.6}$Sr$_{0.4}$FeO$_{3-d}$ composite asymmetric oxygen permeation membranes supported on magnesium oxide

The oxygen permeation through dense Ce$_{0.9}$Gd$_{0.1}$O$_{1.95}$-La$_{0.6}$Sr$_{0.4}$FeO$_{3-d}$ dual-phase composite asymmetric membranes supported on a porous MgO tube was studied. The membranes were prepared by thermoplastic extrusion, dip coating, co-sintering and infiltration of a catalyst. Oxygen permeation measurements and electrical conductivity characterization of the membrane were performed as a function of temperature and oxygen partial pressure. The oxygen flux through the membrane in a H$_2$/air gradient at 850 °C reached 15 N ml cm$^{-2}$ min$^{-1}$. The measured oxygen flux was in good agreement with the theoretically estimated one, taking into account the transport properties of the composite, surface exchange losses, gas diffusion and gas conversion in the MgO support. The performance of the membrane was limited by the surface exchange for the operation in N$_2$/air, CO$_2$/air and H$_2$/air at low temperatures and most probably by the porosity of the MgO support for the operation in H$_2$/air at 850 °C. The stability tests of the membrane in CO$_2$/air and H$_2$/air configurations revealed that an initial degradation of the oxygen flux occurs and it is followed by a relatively stable performance. Post-mortem analysis of the membrane after 900 h of operation did not reveal any significant microstructural degradation of the membrane layer.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Ceramic Engineering & Science, Fundamental Electrochemistry
Authors: Ovtar, S. (Intern), Gurauskis, J. (Intern), Bjøremun Haugen, A. (Intern), Chatzichristodoulou, C. (Intern), Kaiser, A. (Intern), Hendriksen, P. V. (Intern)
Number of pages: 12
Pages: 576-587
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Membrane Science
Volume: 523
ISSN (Print): 0376-7388
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): SNIP 1.898 SJR 2.4 CiteScore 6.93
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 6.13 SJR 2.087 SNIP 1.731
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.978 SNIP 1.763 CiteScore 5.89
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.436 SNIP 1.924 CiteScore 5.42
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.451 SNIP 1.994 CiteScore 5.38
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 2.185 SNIP 1.962 CiteScore 4.37
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
The present report describes a Windows based computer program called PALSfit3. The purpose of the program is to carry out analyses of spectra that have been measured by positron annihilation lifetime spectroscopy (PALS). PALSfit3 is based on the well tested PATFIT and PALS fit programs, which have been used extensively by the positron annihilation community. The present document describes the mathematical foundation of the PALSfit3 model as well as a number of features of the program. The cornerstones of PALSfit3 are two least squares fitting modules: POSITRONFIT and RESOLUTIONFIT. In both modules a model function will be fitted to a measured lifetime spectrum. This model function consists of a function representing the physics of the positron decay which is convoluted with the experimental time resolution function, plus a constant background. The ‘physics function’ consists of a sum of decaying exponentials each of which may be broadened by convolution with a log-normal lifetime distribution. The time resolution function is described by a sum of Gaussians which may be displaced with respect to each other. Various types of constraints may be imposed on the fitting parameters. In the POSITRONFIT module, the fitting parameters to be extracted from a measured spectrum are for each lifetime component its mean lifetime and its broadening as well as its intensity. A correction for positrons annihilating outside the sample can be made as part of the analysis. In the RESOLUTIONFIT module, parameters determining the shape of the time resolution function can be fitted. The extracted resolution function may then be used in POSITRONFIT.

Graphics displays are provided to ease the selection of some of the input parameters and to display results of spectrum analysis. The results are also available in a text window. PALSfit3 is verified on Windows XP and Windows 7, 8 and 10. The PALSfit3 software can be acquired from the Technical University of Denmark (http://PALSfit.dk)

General information
State: Published
Passive characterization and active testing of epoxy bonded regenerators for room temperature magnetic refrigeration

Epoxy bonded regenerators of both spherical and irregular La(Fe,Mn,Si)\textsubscript{13}H\textsubscript{x} particles have been developed aiming at increasing the mechanical strength of active magnetic regenerators (AMR) loaded with brittle magnetocaloric materials and improving the flexibility of shaping the regenerator geometry. Although the magnetocaloric properties of these materials are well studied, the flow and heat transfer characteristics of the epoxy bonded regenerators have seldom been investigated. This paper presents a test apparatus that passively characterizes regenerators using a liquid heat transfer fluid with an oscillating flow at low Reynolds numbers, simulating the hydraulic working conditions in AMRs. Dimensionless parameters, including friction factor, effectiveness and overall Nusselt number, are presented for the epoxy bonded La(Fe,Mn,Si)\textsubscript{13}H\textsubscript{x} regenerators and reference packed particle beds. Moreover, a five-layer AMR based on spherical particles is tested actively in a small reciprocating magnetic refrigerator, achieving a no-load temperature span of 16.8 °C using about 143 g of epoxy-bonded La(Fe,Mn,Si)\textsubscript{13}H\textsubscript{x} materials. Simulations based on a one-dimensional (1D) AMR model are also implemented to validate and analyze the results from the active test.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Vacuumschmelze GmbH & Co. KG
Authors: Lei, T. (Intern), Navickaité, K. (Intern), Engelbrecht, K. (Intern), Barcza, A. (Ekstern), Vieyra, H. (Ekstern), Nielsen, K. K. (Intern), Bahl, C. (Intern)
Pages: 10-19
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Applied Thermal Engineering
Volume: 128
ISSN (Print): 1359-4311
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 4.14 SJR 1.505 SNIP 1.837
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.78 SJR 1.438 SNIP 1.851
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.683 SNIP 1.884 CiteScore 3.32
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.539 SNIP 2.187 CiteScore 3.16
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.466 SNIP 2.469 CiteScore 3.31
Passive heat transfer enhancement in 3D corrugated tube
An innovative hydraulic design was studied for corrugated tube geometry for a heat exchanger. An ellipse based double corrugation was used as a concept of the geometry. The hydraulic diameter (Dh) is maintained over the tube length while the shape of the cross section varies continuously along the flow direction. 38 corrugated tubes with a Dh of 5 mm were studied numerically with corrugation heights from 0.23 to 0.69 mm and corrugation periods from 5 to 50 mm for laminar flow with water. Computational fluid dynamics (CFD) is used as a tool to study the effect of corrugation geometry on heat transfer and fluid flow with a constant wall temperature and total pressure drop. The governing equations for these problems were solved using the Finite Element Method. The results of numerical modelling show significant increase in NTU for double corrugated tubes compared to a circular tube. The friction factor increases with increasing of severity index, which represents the degree of tube roughness.
Pd Nanoparticles-Supported Carbon Nanotube-Encapsulated NiO/MgO Composite as an Enhanced Electrocatalyst for Ethanol Electrooxidation in Alkaline Medium

In this work, an easy method is developed to prepare well-dispersed palladium nanoparticles into the carbon nanotube (CNT) encapsulated NiO/MgO nanocomposite by the chemical reduction method. CNT encapsulated NiO/MgO nanocomposite were prepared by autogenous pressure at elevated temperature (RAPET) method. The Pd/(NiO/MgO-CNT) catalyst was characterized using X-ray diffraction (XRD), scanning electron microscopy (SEM), higher resolution-transmission electron microscopy (HR-TEM), Raman spectroscopy and electrochemical analysis. Electrochemical measurements demonstrate the as synthesized Pd/(NiO/MgO-CNT) catalysts exhibit superior electrochemical performance compare to the commercial Pd/C catalysts. The current densities of the main anodic peak of electrooxidation of ethanol increases sharply for the Pd/(NiO/MgO-CNT) (98.20 mA/cm²), which are ~2.1 times as large as that of Pd/C (47 mA/cm²). The excellent electrochemical performance can be attributed on the one hand to the incorporation of NiO/MgO on palladium on the other hand to the porous tubular morphology of the CNT leads to high dispersion of Pd nanoparticles and also enhances the mass transport of the electrode.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Anna University, SRM University
Authors: Mahendiran, C. (Ekstern), Rajesh, D. (Ekstern), Maiyalagan, T. (Ekstern), Kadirvelayutham, P. (Intern)
Pages: 11438–11444
Publication date: 2017
Main Research Area: Technical/natural sciences

Performance and electrochemical analysis of solid oxide fuel cells based on LSCF-YSZ nano-electrode
NiO-YSZ/YSZ/LSCF-YSZ tri-layer structure SOFC has been fabricated by tape casting and infiltration methods. Subsequently, polarization curves and electrochemical impedance spectra measurement were carried out to evaluate cell performance at 850-700°C with varied steam content in hydrogen supplied to the anode. At 800°C, open circuit voltage for 4% steam-humidified hydrogen reached 1.069 V, along with a power density of 831 mW/cm² at 0.7 V. Furthermore, 500 hours of long-term durability test has been performed at 750°C in hydrogen atmosphere, as a consequence that a voltage degradation rate of 1.7%/kh has been measured.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Tsinghua University
Authors: Jia, C. (Ekstern), Chen, M. (Intern), Han, M. (Ekstern)
Pages: 1006-1012
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: International Journal of Applied Ceramic Technology
Volume: 14
Issue number: 5
ISSN (Print): 1546-542X
Ratings:
Web of Science (2018): Indexed yes
Scopus rating (2017): CiteScore 1.21 SJR 0.378 SNIP 0.684
Performance Improvement of an Inhomogeneous Cathode by Infiltration

The performance of solid oxide fuel cells (SOFCs) is considerably influenced by the microstructure and chemical composition of cathode materials. Porous La$_{0.85}$Sr$_{0.15}$FeO$_3$–Ce$_{0.9}$Gd$_{0.1}$O$_2$ composite electrodes were infiltrated by La$_{0.6}$Sr$_{0.4}$CoO$_3$ and La$_{0.6}$Sr$_{0.4}$FeO$_3$. The effects of infiltration loading, calcination temperature of infiltrated material and co-infiltration of LSC and LSF were investigated using electrochemical impedance measurement, microstructural analysis, and high-temperature X-ray diffraction (HT-XRD). A symmetrical cell two-electrode configuration was used to examine the electrochemical performance of the electrodes. The electrochemical results revealed that the polarization resistance of the cathodes significantly was decreased by infiltration from 2.59 to 0.034 Ω cm$^2$ measured at 670 °C. The best electrode performance was achieved at a calcination temperature of 770 °C. It was also found that infiltration of LSC improved the stability of the electrodes during 145 h of testing at 620 °C in air at open circuit voltage (OCV).
An electrochemical reactor can be used to purify flue gasses. Such a reactor can be a multilayer structure consisting of alternating layers of porous electrodes and electrolytes (a porous cell stack). In this work optimization of such a unit has been done by changing the pore former composition and the electrode powder pre-treatment. The effect on permeability, mechanical strength and electrochemical behavior was studied in this work. The effects were evaluated by measuring the pressure difference over the samples in relation to the flow through the sample, by the ball on ring method and by...
Electrochemical impedance spectroscopy in air at temperatures between 300 and 450 °C. The resulting structures were also evaluated with scanning electron microscopy. The work showed a dependence on the pore former composition and electrode powder pre-treatment resulting in variations in porosity, strength and flow resistance. A higher porosity gives a lower backpressure. The electrochemical performance shows that both thickness and amount of pore former in the electrolyte is important, but almost no dependence of electrode composition on the polarization resistances within the tested compositions.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Mixed Conductors
Authors: Andersen, K. B. (Intern), Charlas, B. (Intern), Stamate, E. (Intern), Kammer Hansen, K. (Intern)
Number of pages: 22
Publication date: 2017
Main Research Area: Technical/natural sciences

Phonon thermal conductivity of scandium nitride for thermoelectrics from first-principles calculations and thin-film growth
The knowledge of lattice thermal conductivity of materials under realistic conditions is vitally important since many modern technologies require either high or low thermal conductivity. Here, we propose a theoretical model for determining lattice thermal conductivity, which takes into account the effect of microstructure. It is based on ab initio description that includes the temperature dependence of the interatomic force constants and treats anharmonic lattice vibrations. We choose ScN as a model system, comparing the computational predictions to the experimental data by time-domain thermoreflectance. Our experimental results show a trend of reduction in lattice thermal conductivity with decreasing domain size predicted by the theoretical model. These results suggest a possibility to control thermal conductivity by microstructural tailoring and provide a predictive tool for the effect of the microstructure on the lattice thermal conductivity of materials based on ab initio calculations.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, National University of Singapore, Linköping University
Authors: Kerdsongpanya, S. (Ekstern), Hellman, O. (Ekstern), Sun, B. (Ekstern), Koh, Y. K. (Ekstern), Lu, J. (Ekstern), Van Nong, N. (Intern), Simak, S. I. (Ekstern), Alling, B. (Ekstern), Eklund, P. (Ekstern)
Number of pages: 6
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Heliyon
Volume: 3
Article number: e00371
ISSN (Print): 2405-8440
Ratings:
Scopus rating (2017): CiteScore 1.23 SJR 0.355 SNIP 0.572
Scopus rating (2016): CiteScore 0.62 SJR 0.187 SNIP 0.72
Original language: English
Chemical engineering, Materials science
Electronic versions:
DOIs:
10.1016/j.heliyon.2017.e00371
Source: FindIt
Source-ID: 2373600545
Publication: Research - peer-review › Journal article – Annual report year: 2017

Publication information
Journal: Physical Review B
Volume: 96
Issue number: 19
Article number: 195417
ISSN (Print): 2469-9950
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Plasma and catalyst for the oxidation of NOx

The removal of NOx from the exhaust gases requires the oxidation of most abundant NO to NO2 or N2O5. The oxidation can be done by non-thermal plasma but the efficiency is limited due to the back-reaction of NO2 to NO by O radicals. Present contribution investigates the role of catalysts in the improvement of oxidation efficiency based on the stationary and time-dependent studies of the NOx oxidation at different reactor configurations and experimental conditions. The plasma produced active oxygen species (O, O3) were shown to play an important role in the reactions taking place on the catalyst surfaces while the exact mechanism and extent of the effect depended on the reactor configuration. The effect of
catalyst at different experimental conditions was quantitatively described with the aid of analytical lumped kinetic models derived for the NOx oxidation when the catalyst was directly in contact with plasma or only with the ozone.

**General information**
State: Published
Organisations: Department of Energy Conversion and Storage, University of Tartu
Authors: Jögi, I. (Ekstern), Erme, K. (Ekstern), Levoll, E. (Ekstern), Raud, J. (Ekstern), Stamate, E. (Intern)
Pages: 32
Publication date: 2017

**Host publication information**
Title of host publication: Proceedings of the XXXIII International Conference on Phenomena in Ionized Gases (ICPIG 2017)
Main Research Area: Technical/natural sciences
Conference: 33rd International Conference on Phenomena in Ionized Gases (ICPIG 2017), Estoril, Portugal, 09/07/2017 - 09/07/2017
Electronic versions: ICPIG2017_proceedings_32.pdf
Source: PublicationPreSubmission
Source-ID: 142691215
Publication: Research - peer-review › Article in proceedings – Annual report year: 2018

**Potential- and Rate-Determining Step for Oxygen Reduction on Pt(111)**
Using density functional theory calculations, we study reaction thermodynamics and kinetics for the oxygen reduction reaction (ORR) on surface coverages that develop in the 0 – 1.0 V potential range on Pt(111), with special emphasis on the role of water. At low potentials, water affects adsorption energies of hydrophilic *O2 and *OOH intermediates but displays a limited effect on the transition state energies for their dissociation. We calculate the O2 and OOH adsorption and dissociation free energies at most stable surfaces in the investigated potential range and arrive at two important conclusions 1) the ORR proceeds through the associative reaction mechanism in the diffusion and the mixed kinetic-diffusion region and 2) moderate O2 and OOH activation energies support the notion that the reaction is predominantly controlled by the rate prefactor. We associate the rate prefactor with the probability for an O2 molecule to replace a water molecule on hydrophilic (OH - H2O covered) surfaces, and the inability of O2 to adsorb and dissociate on hydrophobic (O covered) surfaces that develop at higher potentials. Finally, in light of new results, we discuss activities of Pt alloys that lie close to the top of the volcano.

**General information**
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials
Authors: Tripkovic, V. (Intern), Vegge, T. (Intern)
Pages: 26785–26793
Publication date: 2017
Main Research Area: Technical/natural sciences

**Publication information**
Journal: Journal of Physical Chemistry C
Volume: 121
Issue number: 48
ISSN (Print): 1932-7447
Ratings: BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 4.58 SJR 2.135 SNIP 1.147
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.48 SJR 1.964 SNIP 1.195
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.886 SNIP 1.26 CiteScore 4.68
Web of Science (2015): Indexed yes
Potential for dynamic pricing in district heating systems in Denmark and Finland

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Centre for IT-Intelligent Energy Systems in Cities, Aalto University
Authors: Dominkovic, D. F. (Intern), Wahlroos, M. (Ekstern), Syri, S. (Ekstern), Pedersen, A. S. (Intern)
Number of pages: 1
Publication date: 2017

Host publication information
Main Research Area: Technical/natural sciences

Relations
Projects:
Potential of district cooling in hot and humid climates

Efficiently utilizing energy that is currently being wasted can significantly increase energy efficiency of the system, as well as reduce the carbon footprint. In hot climates with large cooling demands, excess waste heat can be utilized via absorption chillers to generate cold. Moreover, cold from liquefied natural gas gasification process can further provide energy source for meeting the cold demand. In order to connect the large sources of waste heat and cold energy with customers demanding the cold, a significant investment in district cooling grid is a necessity. In order to deal with the mentioned issue, an existing energy balance model was complemented with Matlab algorithms in order to model the whole energy system, including the detailed representation of the district cooling grid. Singapore was chosen for a case study and several different scenarios were developed for the year 2050, with the main indicators being total primary energy supply, total CO₂ emissions and total socio-economic costs. The most beneficial scenario for the year 2050 had 19.5% lower primary energy demand, 38.4% lower total socio-economic costs and 41.5% lower CO₂ emissions compared to the business-as-usual scenario for the year 2050, although significant investment in the district cooling grid was included in the calculations.
Potential Of Waste Heat And Waste Cold Energy Recovery In Singapore For District Cooling Applications: Impacts On Energy System

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Centre for IT-Intelligent Energy Systems in Cities, Nanyang Technological University, IMechE
Authors: Dominkovic, D. F. (Intern), Romagnoli, A. (Ekstern), Fox, T. (Ekstern), Pedersen, A. S. (Intern)
Number of pages: 2
Publication date: 2017

Host publication information
Title of host publication: Proceedings of the 40th IAEE International Conference - Extended abstracts : Meeting the Energy Demands of Emerging Economies
Publisher: IAEE
Main Research Area: Technical/natural sciences
Conference: 40th Annual IAEE International Conference, Singapore, Singapore, 18/06/2017 - 18/06/2017
Electronic versions:
Extended_Abstract_Potential_of_waste_heat_and_waste_cold_energy_recovery_in_Singapore_for_district_cooling_applications.pdf
Links:
https://www.iaee.org/proceedings/article/14390

Pressurized reversible operation of a 30-cell solid oxide cell stack using carbonaceous gases
Recent theoretical studies show that reversible electrochemical conversion of H2O and CO2 to CH4 inside pressurized solid oxide cells (SOCs) combined with subsurface storage of the produced gases can facilitate seasonal electricity
storage with a round-trip efficiency reaching 70-80% and a storage cost below 3 ¢/kWh. Here we show test results with a 30-cell SOFCMAN 301 stack operated with carbonaceous gases at 18.7 bar and 700 °C in both electrolysis and fuel cell mode. The CH4 content in the stack outlet gas increased from 0.22% at open circuit voltage (OCV) to 18% at -0.17 A cm-2 in electrolysis mode. The degradation rates in both fuel cell and electrolysis mode were comparable to previously reported SOFCMAN stack degradation rates measured at ambient pressure operation with H2/H2O gas mixtures.

**General information**
State: Published
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry, Mixed Conductors, Department of Mechanical Engineering, Thermal Energy, Technical University of Denmark
Authors: Jensen, S. H. (Intern), Langnickel, H. (Intern), Hintzen, N. (Ekstern), Chen, M. (Intern), Sun, X. (Intern), Hauch, A. (Intern), Butera, G. (Intern), Clausen, L. R. (Intern)
Pages: 413-414
Publication date: 2017

**Host publication information**
Title of host publication: Proceedings of the 7th European Fuel Cell Technology & Applications Conference (EFC2017)
Publisher: ENEA
Article number: EFC17255 EFC17
ISBN (Print): 978-88-8286-324-1
Main Research Area: Technical/natural sciences
Conference: 7th European Fuel Cell Technology & Applications Conference (EFC2017), Naples, Italy, 12/12/2017 - 12/12/2017
Pressure, Internal, Methane, Efficiency, Storage
Electronic versions:
EFC17255_Full_paper_20171118_revised_updated_FC_GC_Fig.pdf
Links:
http://www.europeanfuelcell.it/images/proceedings_EFC17.pdf
Publication: Research - peer-review › Article in proceedings – Annual report year: 2017

Printed organic smart devices characterized by nonlinear optical
In this study, we demonstrate that nonlinear optical microscopy is a promising technique to characterize organic printed electronics. Using ultrashort laser pulses we stimulate two-photon absorption in a roll coated polymer semiconductor and map the resulting two-photon induced photoluminescence (TPPL) and second harmonic response. First, we show that the different nonlinear optical signals can be used to discriminate between the polymer semiconductor material and embedded metal nanoparticles which constitute the electrode in a real device. Next we demonstrate that the TPPL quenches when applying a current between source and drain; this decrease can be used to determine the electrical characteristic of the device [1]. Finally, we show that the TPPL increases with higher temperature in the 20 - 120 °C range, closely following the supported current characteristics of the semiconductor. With this technique, we can recognize different nanomaterials and we propose that the TPPL is a good indicator to map and monitor the charge carrier density and the molecular packing of the printed polymer material. Importantly, simple calculations based on the signal levels, suggest that this technique can be extended to the real time mapping of the polymer semiconductor film, even during the printing process, in which the high printing speed poses the need for equally high acquisition rates.

**General information**
State: Published
Organisations: Department of Energy Conversion and Storage, Organic Energy Materials, Institut de Ciències Fotòniques, Catalan Institution for Research and Advanced Studies
Authors: Pastorelli, F. (Intern), Accanto, N. (Ekstern), Jørgensen, M. (Intern), van Hulst, N. F. (Ekstern)
Pages: 38
Publication date: 2017

**Host publication information**
Title of host publication: PLASMONICA 2017: Book of Abstracts
Article number: T19
Main Research Area: Technical/natural sciences
Workshop: 5th International Workshop on Plasmonics (PLASMONICA 2017), Lecce, Italy, 05/07/2017 - 05/07/2017
Electronic versions:
Links:
http://www.plasmonica2017.it/
Source: PublicationPreSubmission
Source-ID: 134441400
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2017
Printed organic smart devices characterized by ultra-short laser pulses

Resume: In this study, we demonstrate that nonlinear optical microscopy is a promising technique to characterize organic printed electronics. Using ultrashort laser pulses we stimulate two-photon absorption in a roll coated polymer semiconductor and map the resulting two-photon induced photoluminescence (TPPL) and second harmonic response. First, we show that the different nonlinear optical signals can be used to discriminate between the polymer semiconductor material and embedded nanoparticles which constitute the electrode in a real device. Next we demonstrate that the TPPL quenches when applying a current between source and drain; this decrease can be used to determine the electrical characteristic of the device. Finally, we show that the TPPL increases with higher temperature in the 20 - 120 °C range, closely following the supported current characteristics of the semiconductor. We propose that the TPPL is a good indicator to map and monitor the charge carrier density and the molecular packing of the printed polymer material. Importantly, simple calculations based on the signal levels, suggest that this technique can be extended to the real time mapping of the polymer semiconductor film, even during the printing process, in which the high printing speed poses the need for equally high acquisition rates.

Probing phosphoric acid redistribution and anion migration in polybenzimidazole membranes

Micro platinum electrodes embedded in a laminated phosphoric acid doped polybenzimidazole membrane are employed to monitor the acid migration during hydrogen pump mode operation. Upon application of a constant current, an immediate ohmic resistance decrease of the membrane near the anode is observed, accompanied by a corresponding increase near the cathode side. This is a direct evidence of migration of the acid anions via the vehicle conducting mechanism, resulting in an accumulation of acid at the anode side and depletion at the cathode side. Both resistances reach a steady state value after a prolonged period of measurement, apparently balanced by the back diffusion of the acid molecules. The phenomenon is magnified at higher current densities and with increased thickness of the overall membrane, which is of significance in quantitative understanding of the proton conductivity mechanism e.g. for determination of the anionic transference number. The finding provides a technique to monitor the acid redistribution within the membrane as a basis for an engineering solution to address the long-term durability of fuel cells built around phosphoric acid doped polymer membranes.
Production and Reliability Oriented SOFC Cell and Stack Design

General information
State: Published
Production and Reliability Oriented SOFC Cell and Stack Design

The paper presents an innovative development methodology for a production and reliability oriented SOFC cell and stack design aiming at improving the stacks robustness, manufacturability, efficiency and cost. Multi-physics models allowed a probabilistic approach to consider statistical variations in production, material and operating parameters for the optimization phase. A methodology for 3D description of spatial distribution of material properties based on a random field models was developed and validated by experiments. Homogenized material models on multiple levels of the SOFC stack were established. The probabilistic models were related to the experimentally obtained properties of base materials to establish a statistical relationship between the material properties and the most relevant load effects. Software algorithms for meta models that allow the detection of relationships between input and output parameters and to perform a sensitivity analysis were developed and implemented. The capabilities of the methodology is illustrated on two practical cases.
Progress of SOFC/SOEC Development at DTU Energy: From Materials to Systems

DTU Energy has over the past 20 years had a very substantial effort on SOFC/SOEC development. The current project volume corresponds to ~40 man years per year. Activities span over a broad range in the value chain, from materials to cells, stacks and analyses at energy system level. In addition to that, research areas comprise ceramic processing methods, micro-structural analysis, electrochemical characterization, and modelling. Among recent highlights are electrode and cell developments, including metal supported cells, stack development durability studies under realistic operation conditions and stack operation at high pressure.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry, Mixed Conductors
Authors: Hagen, A. (Intern), Hendriksen, P. V. (Intern)
Number of pages: 9
Pages: 145-153
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: E C S Transactions
Volume: 78
Issue number: 1
ISSN (Print): 1938-5862
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 0.44 SJR 0.225 SNIP 0.252
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 0.4 SJR 0.228 SNIP 0.253
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.211 SNIP 0.244 CiteScore 0.36
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.212 SNIP 0.234 CiteScore 0.36
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.192 SNIP 0.231 CiteScore 0.27
ISI indexed (2013): ISI indexed no
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.241 SNIP 0.26 CiteScore 0.29
ISI indexed (2012): ISI indexed no
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.261 SNIP 0.28 CiteScore 0.36
ISI indexed (2011): ISI indexed no
Pulsed Laser Deposition of $\text{YBa}_2\text{Cu}_3\text{O}_{x}$ with Scanning Beam: Target to Substrate Composition Transfer and Film Structure

Pulsed laser deposition is often considered a process providing congruent transfer of target composition to the growing film. In fact, many different processes affect compositional preservation, starting from incongruent target ablation, to scattering on the way to the substrate, and to processes of the film formation on the substrate surface. We developed a pulsed laser deposition process trying to minimize the compositional deviations due to the scattering by the ambient gas by applying laser beam scanning across the target surface and substitution of oxygen with argon in the chamber during deposition. Transfer of elemental composition of $\text{YBa}_2\text{Cu}_3\text{O}_7$ targets with compositions varying from stoichiometric 1/2/3 ratio was tested by deposition of thin films in conditions optimal for high-temperature superconductor formation. Despite all measures, the films still show Ba,Y enrichment due to different efficiencies of scattering on the ambient gas. The Y part in the film followed well the composition of the target, but the Ba enrichment was almost constant for most of the studied target compositions, implying a crucial role of the film growth processes. The $\text{YBa}_2\text{Cu}_3\text{O}_{x}$ (YBCO) films show a layered structure, with increased density of defects in the topmost layer. We suppose this is due to expelling of the excess Ba into the top layer with formation of a quasi-liquid layer promoting formation of a high-density YBCO film.
Pulsed laser deposition (PLD) of the CZTS absorber for thin solar cells with up to 5.2-% -efficiency

General information
State: Published
Organisations: Department of Photonics Engineering, Photovoltaic Materials and Systems, DTU Danchip, Department of Energy Conversion and Storage, Electrofunctional materials, Applied Electrochemistry, Department of Physics, Experimental Surface and Nanomaterials Physics, Silicon Microtechnology, Department of Micro- and Nanotechnology, University of New South Wales
Authors: Cazzaniga, A. C. (Intern), Canulescu, S. (Intern), Ettlinger, R. B. (Intern), Pryds, N. (Intern), Hansen, O. (Intern), Schou, J. (Intern), Crovetto, A. (Intern), Hansen, O. (Intern), Yan, C. (Ekstern), Sun, K. (Ekstern), Hao, X. (Ekstern)
Number of pages: 1
Publication date: 2017
Event: Abstract from EMRS Spring meeting 2017, Strasbourg, France.
Main Research Area: Technical/natural sciences
Electronic versions:
Abstract_Earth_abundant_CZTS.pdf
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2017

Pulsed laser deposition (PLD) of the CZTS absorber for thin solar cells with up to 5.2-% -efficiency

General information
Quality Assurance of Solid Oxide Fuel Cell (SOFC) and Electrolyser (SOEC) Stacks

In the EU-funded project “Solid oxide cell and stack testing and quality assurance” (SOCTESQA) standardized and industry wide test modules and programs for high temperature solid oxide cells and stacks are being developed. These test procedures can be applied for the fuel cell (SOFC), the electrolysis (SOEC) and in the combined SOFC/SOEC mode. In order to optimize the test modules the project partners have tested identical SOx stacks with the same test programs in several testing campaigns. Altogether 10 pre-normative test modules were developed: Start-up, current-voltage characteristics, electrochemical impedance spectroscopy, reactant utilization, reactant gas composition, temperature sensitivity, operation at constant current, operation at varying current, thermal cycling and shut-down. The test modules were validated by comparing the results in terms of repetitiveness of the different testing campaigns and in terms of reproducibility among the different partners. Moreover, the results are discussed in context to the test input parameters.

General information

State: Published
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry, German Aerospace Center (DLR), Grenoble-Alpes University, Italian National Agency for New Technologies, European Commission Joint Research Centre Institute, European Institute for Energy Research, Nanyang Technological University
Authors: Lang, M. (Ekstern), Auer, C. (Ekstern), Couturier, K. (Ekstern), Sun, X. (Intern), McPhail, S. J. (Ekstern), Malkow, T. (Ekstern), Fu, Q. (Ekstern), Liu, Q. (Ekstern)
Number of pages: 10
Pages: 2077-2086
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: E C S Transactions
Volume: 78
Issue number: 1
ISSN (Print): 1938-5862
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 0.44 SJR 0.225 SNIP 0.252
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 0.4 SJR 0.228 SNIP 0.253
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.211 SNIP 0.244 CiteScore 0.36
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.212 SNIP 0.234 CiteScore 0.36
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.192 SNIP 0.231 CiteScore 0.27
ISI indexed (2013): ISI indexed no
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.241 SNIP 0.26 CiteScore 0.29
Quantification of solar cell failure signatures based on statistical analysis of electroluminescence images

We propose a method to identify and quantify the extent of solar cell cracks, shunting, or damaged cell interconnects, present in crystalline silicon photovoltaic (PV) modules by statistical analysis of the electroluminescence (EL) intensity distributions of individual cells within the module. From the EL intensity distributions (ELID) of each cell, we calculated summary statistics such as standard deviation, median, skewness and kurtosis, and analyzed how they correlate with the type of the solar cell degradation.

We found that the dispersion of the ELID increases with the size and severity of the solar cell cracks, correlating with an increase in standard deviation and decrease in kurtosis. For shunted cells, we found that the ELID median is strongly correlated with the extent of cell shunting. Last, cells with damaged interconnect ribbons show current crowding and increased series resistance regions, characterized by increased dispersion and skewness of the ELID. These cell-level diagnostic parameters can be used to quantify the level of mismatch between the solar cells in the module, which can represent the extent of the module degradation, due to transportation, installation, or field operation. The method can be easily automated for quality control by module manufacturers or installers, or can be used as a diagnostic tool by plant operators and diagnostic service providers.

General information
State: Published
Organisations: Department of Photonics Engineering, Photovoltaic Materials and Systems, Organic Energy Materials, Aalborg University, National Renewable Energy Laboratory
Authors: Spataru, S. (Ekstern), Parikh, H. (Ekstern), Benatto, G. A. D. R. (Intern), Hacke, P. (Ekstern), Sera, D. (Ekstern), Poulsen, P. B. (Intern)
Pages: 1466-1472
Publication date: 2017

Host publication information
Title of host publication: Proceedings of 33rd European Photovoltaic Solar Energy Conference and Exhibition
Main Research Area: Technical/natural sciences

Relations
Projects:
Quantification of solar cell failure signatures based on statistical analysis of electroluminescence images
Source: PublicationPreSubmission
Source-ID: 139806368
Publication: Research - peer-review › Article in proceedings – Annual report year: 2017

Quasi-Elastic Neutron Scattering Studies on Solid Electrolytes for solid state Lithium Batteries

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials
Radical production efficiency and electrical characteristics of a coplanar barrier discharge built by multilayer ceramic technology

The present study investigated the electrical characteristics and radical production efficiency of a coplanar barrier discharge (CBD) device manufactured by Kyocera by multilayer ceramic technology. The device consisted of a number of linear electrodes with electrode and gap widths of 0.75 mm, immersed into a ceramic dielectric barrier. A closed flow-through system necessary for the measurements was prepared by placing a quartz plate at a height of 3 mm from the ceramic barrier. The production of nitrogen radicals was determined from the removal of a trace amount of NO in pure N2 gas, while the production of oxygen radicals was determined by ozone production in pure O2 or synthetic air. The production efficiency of N and O radicals and NO oxidation in synthetic air was comparable with the efficiency of a volume barrier discharge device. The power density per unit of surface area of the CBD device was more than two times larger than that of a similar volume barrier discharge setup, which makes the CBD device a compact alternative for gas treatment. The production of ozone and different nitrogen oxides was also evaluated for the open system of the CBD which is usable for surface treatment. The ozone concentration of this system was nearly independent from the input power, while the concentration of nitrogen oxides increased with input power. The open system of the CBD was additionally tested for the treatment of a silicon surface. An increase of applied power decreased the time required to reduce the water contact angle below 10 degrees but also started to have an impact on the surface roughness.
Scopus rating (2012): SJR 1.279 SNIP 1.414 CiteScore 2.31
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.266 SNIP 1.399 CiteScore 2.36
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.292 SNIP 1.28
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.269 SNIP 1.327
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.427 SNIP 1.549
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.38 SNIP 1.612
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.406 SNIP 1.742
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.216 SNIP 1.455
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.133 SNIP 1.438
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 0.912 SNIP 1.221
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 1.033 SNIP 1.233
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.925 SNIP 1.212
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 0.842 SNIP 1.125
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 0.89 SNIP 1.264
Original language: Undefined/Unknown
DOIs: 10.1088/1361-6463/aa8dab
Source: FindIt
Source-ID: 2389647408
Publication: Research - peer-review › Journal article – Annual report year: 2017

Reduction of the thermal conductivity of the thermoelectric material ScN by Nb alloying

ScN-rich (Sc,Nb)N solid solution thin films have been studied, motivated by the promising thermoelectric properties of ScN-based materials. Cubic Sc\textsubscript{1-x}Nb\textsubscript{x}N films for 0 ≤ x ≤ 0.25 were epitaxially grown by DC reactive magnetron sputtering on a c-plane sapphire substrate and oriented along the (111) orientation. The crystal structure, morphology, thermal conductivity, and thermoelectric and electrical properties were investigated. The ScN reference film exhibited a Seebeck coefficient of −45 μV/K and a power factor of 6 × 10\textsuperscript{−4} W/m K\textsuperscript{2} at 750 K. Estimated from room temperature Hall measurements, all samples exhibit a high carrier density of the order of 10\textsuperscript{21} cm\textsuperscript{−3}. Inclusion of heavy transition metals into ScN enables the reduction in thermal conductivity by an increase in phonon scattering. The Nb inserted ScN thin films exhibited a thermal conductivity lower than the value of the ScN reference (10.5 W m\textsuperscript{−1} K\textsuperscript{−1}) down to a minimum value of 2.2 Wm\textsuperscript{−1}K\textsuperscript{−1}. Insertion of Nb into ScN thus resulted in a reduction in thermal conductivity by a factor of ∼5 due to the mass contrast in ScN, which increases the phonon scattering in the material.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Linköping University, Sorbonne Universités, Indian Institute of Technology Mandi
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 2.184 SNIP 1.7
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 2.147 SNIP 1.554
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 2.009 SNIP 1.53
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 1.973 SNIP 1.486

Relation Between Ni Particle Shape Change and Ni Migration in Ni–YSZ Electrodes – a Hypothesis

This paper deals with degradation mechanisms of Ni–YSZ electrodes for solid oxide cells, mainly solid oxide electrolysis cells (SOECs), but also to some extent solid oxide fuel cells (SOFCs). Analysis of literature data reveals that several apparently different and even in one case apparently contradicting degradation phenomena are a consequence of interplay between loss of contact between the Ni–YSZ (and Ni–Ni particles) in the active fine-structured composite fuel electrode layer and migration of Ni via weakly oxidized Ni hydroxide species. A hypothesis that unravels the apparent contradiction and explains qualitatively the phenomena is presented, and as a side effect, light has been shed on a degradation phenomenon in solid oxide fuel cells (SOFCs) that has been observed during a decade.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry, Mixed Conductors
Authors: Mogensen, M. B. (Intern), Hauch, A. (Intern), Sun, X. (Intern), Chen, M. (Intern), Tao, Y. (Intern), Ebbesen, S. D. (Intern), Hansen, K. V. (Intern), Hendriksen, P. V. (Intern)
Pages: 434-441
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Fuel Cells
Volume: 17
Issue number: 4
ISSN (Print): 1615-6846
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 1.88 SJR 0.559 SNIP 0.748
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.79 SJR 0.495 SNIP 0.603
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.685 SNIP 0.779 CiteScore 2.02
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.615 SNIP 0.792 CiteScore 2.05
Web of Science (2014): Indexed yes
Releasing cation diffusion in self-limited nanocrystalline defective ceria thin films

Accepter-doped nanocrystalline cerium oxide thin films are mechanically constrained nano-domains, with film/substrate interfacial strain and chemical doping deadlock mass diffusion. In contrast, in this paper we show that chemical elements result in highly unstable thin films under chemical reduction, with unexpected diffusion-driven effects such as fast migration of grain boundaries, porosity nucleation, and interdiffusion at low temperatures.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Imaging and Structural Analysis, Electrofunctional materials, Chinese Academy of Sciences
Authors: Esposito, V. (Intern), Ni, D. W. (Ekstern), Gualandris, F. (Intern), Pryds, N. (Intern)
Pages: 13784-13788
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: R S C Advances
Volume: 7
Reply to "Comment on 'Performance of Halbach magnet with finite coercivity'"
We reply to Dr. Xu's comment on our paper 'Performance of Halbach magnet arrays with finite coercivity' (JMMM 407 (2016), 369-376). Contrary to Dr. Xu's objections we show that the procedure employed by us correctly accounts for the shape effects of the magnet elements. We show that the partial differential equation for the magnetic vector potential, derived from the Maxwell equations, incorporates all shape effects. On the other hand, the local constitutive relations express a point-wise link between, e.g., magnetic field and magnetic flux density, and are as such independent of geometry. We confirm that the results of our computations are perfectly consistent with the constitutive relation which is assumed as starting point.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Authors: Insinga, A. R. (Intern), Bahl, C. (Intern), Bjørk, R. (Intern), Smith, A. (Intern)
Pages: 386-389
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Magnetism and Magnetic Materials
Volume: 429
ISSN (Print): 0304-8853
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Electronic, Optical and Magnetic Materials, Condensed Matter Physics, Demagnetization, Halbach magnet, Reversal of remanence, Coercive force, Magnetism, Maxwell equations, Constitutive relations, Halbach magnet array, Halbach magnets, Magnetic vector potentials, Point wise, Shape effect, Magnets
Revision of the qualification framework at the Technical University of Denmark Part 2: Applications

Using a revised Qualification Framework (QF) with four main categories: -to know, -to be, -to interact, and -to do, this paper demonstrates how to use the elements of the QF to construct Programme-Qualification Matrices. A general Programme- Qualification Matrix defines the qualifications and their respective conceptual understanding common to all engineering programmes. This is complemented by programme-specific qualification matrices with added emphasis on content and context. Redesigned educational outcomes for three bachelor programmes are presented to demonstrate the versatility of the concept.

Role of the Band Gap for the Interaction Energy of Coadsorbed Fragments

Understanding the interaction between adsorbants and metal surfaces has led to descriptors for bindings and catalysis which have a major impact on the design of metal catalysts. On semiconductor oxides, these understandings are still lacking. We show an important element in understanding binding on semiconductors. We propose here a correlation between the cooperative interaction energy, i.e., the energy difference between the adsorption energies of coadsorbed electron donor–acceptor pair and isolated fragments and the band gap of the clean oxide surface. We demonstrate this effect for a number of oxides and donor–acceptor pairs and explain it with the shift in the Fermi level before and after the adsorption. The conclusion is that the adsorption of acceptor–donor pairs is considerably more favorable compared to unpaired fragments, and this energy difference is approximately equal to the value of the band gap. The implications of this understanding in relation to the improvement and discovery of novel catalysts on the band gap oxides are also discussed.
Scavenging of oxygen vacancies at modulation-doped oxide interfaces: Evidence from oxygen isotope tracing
The introduction of manganite buffer layers, La7/8Sr1/8MnO3 (LSMO) in particular, at the metallic interface between SrTiO3 (STO) and another band insulator suppresses the carrier density of the interfacial two-dimensional electron gas (2DEG) and improves significantly the electron mobility. However, the mechanisms underlying the extreme mobility enhancement remain elusive. Herein, we used 18O isotope exchanged SrTi18O3 as substrates to create 2DEG at room temperature with and without the LSMO buffer layer. By mapping the oxygen profile across the interface between STO18 and disordered LaAlO3 or yttria-stabilized zirconia (YSZ), we provide unambiguous evidence that redox reactions occur at oxide interfaces even grown at room temperature. Moreover, the manganite buffer layer not only suppresses the carrier density but also strongly suppresses the oxygen exchange dynamics of the STO substrate, which likely prevents the
reduction of STO during the formation of the 2DEG. The underlying mechanism on the enhanced electron mobility at buffered oxide interfaces is also discussed.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, ETH Zurich, Paul Scherrer Institut
Authors: Chen, Y. (Intern), Döbeli, M. (Ekstern), Pomjakushina, E. (Ekstern), Gan, Y. (Intern), Pryds, N. (Intern), Lippert, T. (Ekstern)
Number of pages: 6
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Physical Review Materials
Volume: 1
Issue number: 5
Article number: 052002
ISSN (Print): 2475-9953
Original language: English
Electronic versions:
Paper_Yunzhong_Scavenging_of_oxygen_vacancies_revised_final_001_revised_002_.pdf
DOIs:
10.1103/PhysRevMaterials.1.052002
Publication: Research - peer-review › Journal article – Annual report year: 2017

Screening the electrochemical activity of transition metal nanoparticles for SOFC anode infiltration

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Montana State University
Authors: Drasbæk, D. B. (Intern), Traulsen, M. L. (Intern), Walker, R. (Ekstern), Holtappels, P. (Intern)
Number of pages: 1
Publication date: 2017
Event: Abstract from 11th International Symposium on Electrochemical Impedance Analysis (EIA 2017), Camogli, Genova, Italy.
Main Research Area: Technical/natural sciences
Electronic versions:
Abstract_for_EIA11.pdf
Source: PublicationPreSubmission
Source-ID: 140852924
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2017

Secondary creep of porous metal supports for solid oxide fuel cells by a CDM approach
The creep behaviour of porous iron-chromium alloy used in solid oxide fuel cells (SOFCs) becomes relevant under SOFC operating temperatures. In this paper, the secondary creep stage of infiltrated and non-infiltrated porous metal supports (MS) was investigated and theoretically modelled by a continuum damage mechanics (CDM) approach. The behaviour of the porous metal support, in the range from 1 to 17MPa and temperatures between 650 and 700°C, was combined and compared with data from literature of Crofer® 22 APU, taken as zero porosity reference material. The variation of the elastic modulus as function of temperature, determined by the high temperature impulse excitation technique, was directly used to account for the porosity and the related effective stress acting during the creep tests. The proposed creep rate formulation was used to extend the Crofer® 22 APU Monkman-Grant diagram in the viscous creep regime. The influence of oxide scale formation on creep behaviour of the porous MS was assessed by comparing the creep data of pre-oxidised samples tested in reducing atmosphere.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, University of Naples Federico II
Authors: Esposito, L. (Ekstern), Boccaccini, D. N. (Intern), Pucillo, G. P. (Ekstern), Frandsen, H. L. (Intern)
Pages: 155-161
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
SOFC Operation with Real Biogas

Biogas is a valuable energy source and will be available in future in systems relying on renewables. It is an attractive fuel for solid oxide fuel cells (SOFC), which are able to utilize the carbon contained in the biogas and which produce electricity with high efficiency. In the current paper, state-of-the-art SOFCs were studied regarding performance and durability in relation to biogas as fuel and considering important contaminants, specifically sulfur. First, the catalytic behavior in relevant synthetic biogas mixtures was studied and the potential of dry reforming was demonstrated. Successful long term operation of an SOFC under both, conditions of steam and dry reforming, i.e., addition of steam or CO2 to avoid carbon formation was shown. For the steam reforming case a remarkable period of 3,500 h, hereof 3,000 h in the presence of H2S was achieved. Finally, a real biogas from a landfill gas unit was used as fuel. The concept of dry reforming was realized. The SOFC was successfully operated with and in one case even without a specific gas cleaning unit.
Solder free joining as a highly effective method for making contact between thermoelectric materials and metallic electrodes

Quality of joining and interfacial evolution behavior play a critical role in the performance and reliability of thermoelectric (TE) devices. In this study, different joining methods using Zn−2AlZn−2Al solder alloy (1) and solder-free joining with microlayers of Ti and Cr as interconnecting agents (2) were systematically investigated and demonstrated on the low-cost ZnSb TE system. ZnSb material, which was chosen to bond with Ag and Ni metallic electrodes, exhibited a maximum zT value of 0.8 at 400°C. With the joining method (1), Zn from the Zn−2AlZn−2Al solder was found to diffuse/react with both Ag and Ni electrodes, and penetrate into ZnSb legs. SEM-EDX analysis recorded a significant excess of Zn in the ZnSb leg after joining. We found that, using microlayers of Ti and Cr as interconnecting agent, a very good interfacial contact was obtained, and the starting composition of ZnSb legs was preserved. The interfacial contact of ZnSb/Cr/NiZnSb/Cr/Ni was found to be stable after heat treatment at 400°C for 30 h, suggesting solder-free joining as an effective method for reliable contacts in TE devices in the medium temperature region (200°C−400°C).

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Electrofunctional materials
Authors: Malik, S. A. (Intern), Le, T. H. (Intern), Van Nong, N. (Intern)
Pages: 305-311
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Materials Today Energy
Volume: 5
ISSN (Print): 2468-6069
Ratings:
Scopus rating (2017): CiteScore 4.2 SJR 1.621 SNIP 0.733
Original language: English
Low-cost thermoelectrics, Contact resistance, Interface kinetics, Zinc antimonide
DOIs:
10.1016/j.mtener.2017.07.012
Source: PublicationPreSubmission
Source-ID: 134231803
Spatially resolved modelling of inhomogeneous materials with a first order magnetic phase transition

We present a numerical model that can simulate a magnetocaloric sample on the grain size level, including magnetostatics, heat transfer, local hysteresis and spatial variation of stoichiometry expressed as a variation in Curie temperature. Grain structure of a sample is realised as a number of regions each having a uniform and defined through a Voronoi-map. We show that demagnetising effects, caused by a finite sample size, and spatial variation in can account for the previously experimentally observed 'virgin' effects in the adiabatic temperature change and isothermal entropy change, respectively and first order reversal effect as a function of temperature. We conclude that even a very little variation in local stoichiometry of less than a percent, corresponding to a standard deviation in of for has a significant impact on the overall properties and history dependence of a sample.
Spinel-based coatings for metal supported solid oxide fuel cells

Metal supports and metal supported half cells developed at DTU are used for the study of a solution infiltration approach to form protective coatings on porous metal scaffolds. The metal particles in the anode layer, and sometimes even in the support may undergo oxidation in realistic operating conditions leading to severe cell degradation. Here, a controlled oxidation of the porous metal substrate and infiltration of Mn and/or Ce nitrate solutions are applied for in situ formation of protective coatings. Our approach consists of scavenging the FeCr oxides formed during the controlled oxidation into a continuous and well adhered coating. The effectiveness of coatings is the result of composition and structure, but also of the microstructure and surface characteristics of the metal scaffolds.

General information
Spray pyrolysis of doped-ceria barrier layers for solid oxide fuel cells

Gadolinium doped ceria (Ce0.8Gd0.2O2−x-CGO) layer fabricated by spray pyrolysis is investigated as the diffusion barrier for solid oxide fuel cell. It is deposited between the La0.6Sr0.4FeO3−δ cathode and the yttria stabilized zirconia electrolyte to mitigate harmful interdiffusion of elements. The parameters of the fabrication process are linked to the measured area specific resistances of the symmetrical cells and the efficiency of the fuel cells. Results show, that application of 800 Å thick barrier effectively hinder negative reactions, while 400 Å thick layer is sufficient to prevent degradation of the Ohmic resistance.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Gdansk University of Technology
Authors: Szymczewska, D. (Ekstern), Chrzan, A. (Ekstern), Karczewski, J. (Ekstern), Molin, S. (Intern), Jasinski, P. (Ekstern)
Pages: 168-176
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Surface and Coatings Technology
Volume: 313
ISSN (Print): 0257-8972
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 3.08 SJR 0.928 SNIP 1.545
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.56 SJR 0.882 SNIP 1.379
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.852 SNIP 1.37 CiteScore 2.46
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.983 SNIP 1.652 CiteScore 2.44
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.048 SNIP 1.832 CiteScore 2.58
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.041 SNIP 1.641 CiteScore 2.2
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.041 SNIP 1.85 CiteScore 2.38
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.145 SNIP 1.653
Web of Science (2010): Indexed yes
Stability and performance of robust dual-phase \((\text{ZrO}_2)_{0.89}(\text{Y}_2\text{O}_3)_{0.01}(\text{Sc}_2\text{O}_3)_{0.010.10-\text{Al}}_{0.02-\text{Zn}}_{0.98}\text{O}_{1.01}\) oxygen transport membranes

Dual-phase composite oxygen transport membranes consisting of 50 vol\% \(\text{Al}_{0.02}\text{Zn}_{0.98}\text{O}_{1.01}\) and 50 vol\% \((\text{ZrO}_2)_{0.89}(\text{Y}_2\text{O}_3)_{0.01}(\text{Sc}_2\text{O}_3)_{0.010.10-\text{Al}}_{0.02-\text{Zn}}_{0.98}\text{O}_{1.01}\) were successfully developed and tested. The applicability of the membrane in oxy-fuel power plants schemes involving direct exposure to flue gas was evaluated by exposing the membrane to gas streams containing \(\text{CO}_2\), \(\text{SO}_2\), \(\text{H}_2\text{O}\) and investigating possible reactions between the membrane material and these gases. The analyses of the exposed composites by x-ray diffraction (XRD), x-ray fluorescence (XRF), attenuated total reflection Fourier transform infrared spectroscopy (ATR-FTIR), and Raman spectroscopy revealed excellent stability. Additionally, an electrical conductivity measurement over 900 h confirmed that the composite is stable under prolonged exposure to \(\text{CO}_2\). However, an instability of the dual-phase membrane under oxygen partial pressures below \(~10^{-4}\) atm. was found. Oxygen permeation tests on a 1 mm thick self-standing membrane resulted in an oxygen flux of 0.33 mL min\(^{-1}\) cm\(^{-2}\) at 925 °C in air/\(\text{N}_2\). Stability tests in \(\text{CO}_2\) with 3 vol\% \(\text{O}_2\) demonstrated the potential for the use of 10Sc1YSZ-AZO dual-phase membranes in oxy-combustion processes involving direct exposure to flue gas.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Ceramic Engineering & Science, Imperial College London
Pages: 18-27
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Membrane Science
Volume: 543
ISSN (Print): 0376-7388
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): SNIP 1.898 SJR 2.4 CiteScore 6.93
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 6.13 SJR 2.087 SNIP 1.731
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.978 SNIP 1.763 CiteScore 5.89
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.436 SNIP 1.924 CiteScore 5.42
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.451 SNIP 1.994 CiteScore 5.38
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 2.185 SNIP 1.962 CiteScore 4.37
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.823 SNIP 1.715 CiteScore 4.29
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.807 SNIP 1.813
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.635 SNIP 1.689
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.458 SNIP 1.789
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.434 SNIP 1.564
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.819 SNIP 2.441
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.748 SNIP 1.819
Scopus rating (2004): SJR 1.557 SNIP 1.668
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.488 SNIP 1.645
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 1.175 SNIP 1.842
Scopus rating (2001): SJR 1.296 SNIP 1.63
Scopus rating (2000): SJR 1.47 SNIP 1.71
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 1.381 SNIP 1.515
Original language: English
Oxygen transport membrane, Composite membrane, CO 2 stability, SO 2 tolerance, Oxy-fuel combustion
DOIs:
10.1016/j.memsci.2017.08.044
Publication: Research - peer-review › Journal article – Annual report year: 2017
Stability of V$_2$O$_5$ Supported on Titania in the Presence of Water, Bulk Oxygen Vacancies, and Adsorbed Oxygen Atoms

A catalyst consisting of vanadium oxide submonolayers supported on rutile titanium dioxide is used for a variety of reactions. One important question is the difference between the activity of monomeric clusters (having one vanadium atom) and polymeric clusters (having more than one vanadium atom). In the case of oxidative dehydrogenation of alkanes and methanol, the reaction produces water, oxygen vacancies, and hydrogen atoms bound to the surface. For this article we use density functional theory to examine how the presence of these species on the surface affects a V$_2$O$_5$ cluster, which we assume to be a representative of a polymeric species. We find that often the presence of other species on the surface can change the composition of the cluster or break it up into two monomeric clusters.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, University of California
Authors: Kristoffersen, H. H. (Intern), Neilson, H. L. (Ekstern), Buratto, S. K. (Ekstern), Metiu, H. (Ekstern)
Pages: 8444-8451
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: The Journal of Physical Chemistry Part C
Volume: 121
Issue number: 15
ISSN (Print): 1932-7447
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 4.58 SJR 2.135 SNIP 1.147
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.48 SJR 1.964 SNIP 1.195
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.886 SNIP 1.26 CiteScore 4.68
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.032 SNIP 1.447 CiteScore 5.08
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 2.143 SNIP 1.445 CiteScore 5.14
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.529 SNIP 1.461 CiteScore 4.98
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.339 SNIP 1.465 CiteScore 4.92
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 2.462 SNIP 1.362
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 2.158 SNIP 1.427
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.883 SNIP 1.04
Status report on high temperature fuel cells in Poland – Recent advances and achievements

The paper presents recent advances in Poland in the field of high temperature fuel cells. The achievements in the materials development, manufacturing of advanced cells, new fabrication techniques, modified electrodes and electrolytes and applications are presented. The work of the Polish teams active in the field of solid oxide fuel cells (SOFC) and molten carbonate fuel cell (MCFC) is presented and discussed. The review is oriented towards presenting key achievements in the technology at the scale from microstructure up to a complete power system based on electrochemical fuel oxidation. National efforts are covering wide range of aspects both in the fundamental research and the applied research. The review present the areas of (i) novel materials for SOFC including ZrO2-based electrolytes, CeO2-based electrolytes, Bi2O3-based electrolytes and proton conducting electrolytes, (ii) cathode materials including thermal shock resistant composite cathode material and silver-containing composites, (iii) anode materials, (iv) metallic interconnects for SOFC, (v) novel fabrication techniques, (vi) pilot scale SOFC, including electrolyte supported SOFC (ES-SOFC) and anode supported SOFC (AS-SOFC), (vii) metallic supported SOFC (MS-SOFC), (viii) direct carbon SOFC (DC-SOFC), (ix) selected application of SOFC, (x) advances in MCFC and their applications, (xi) advances in numerical methods for simulation and optimization of electrochemical systems.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Institute of Power Engineering
Pages: 4366-4403
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Volume: 42
Issue number: 7
ISSN (Print): 0360-3199
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 4.1 SJR 1.116 SNIP 1.267
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Strategies to design materials for electrochemical energy conversion and storage technologies

General information
State: Published
Organisations: Department of Energy Conversion and Storage
Authors: Holtappels, P. (Intern)
Number of pages: 1
Structural evolution during calcination and sintering of a \((\La_{0.6}\Sr_{0.4})_{0.99}\CoO_{3-\delta}\) nanofiber prepared by electrospinning

Design of 3-dimensional metal oxide nanofibers by electrospinning is being widely explored. However, the impacts of calcination and sintering on the resulting morphology remain unknown. For the first time, \((\La_{0.6}\Sr_{0.4})_{0.99}\CoO_{3-\delta}\) (LSC) nanofiber, which is among the most promising electrode materials for solid oxide fuel cells, was synthesized by sol-gel electrospinning. By elevating the temperature in oxygen using in situ transmission electron microscopy, we discovered the structural transitions from nanofibers to nanotubes and then to nano-pearl strings. This facile and up-scalable method can be widely applied to design metal oxide one-dimensional nanomaterials with precise control in both geometry (nanofiber, nanotube and nano-pearl string) and surface area (by varying grain size).
Study of geometries of active magnetic regenerators for room temperature magnetocaloric refrigeration

Room temperature magnetic refrigeration has attracted substantial attention during the past decades and continuing to increase the performance of active magnetic regenerators (AMR) is of great interest. Optimizing the regenerator geometry and related operating parameters is a practical and effective way to obtain the desired cooling performance. To investigate how to choose and optimize the AMR geometry, a quantitative study is presented by simulations based on a one-dimensional (1D) numerical model. Correlations for calculating the friction factor and heat transfer coefficient are reviewed and chosen for modeling different geometries. Moreover, the simulated impacts of various parameters on the regenerator efficiency with a constant specific cooling capacity are presented. An analysis based on entropy production minimization reveals how those parameters affect the main losses occurring inside the AMR. In addition, optimum geometry and operating parameters corresponding to the highest efficiency for different geometries are presented and compared. The results show that parallel plate and micro-channel matrices show the highest theoretical efficiency, while the packed screen and packed sphere beds are possibly more practical from the application point of view.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, University of Southern Denmark
Study of Operating Parameters for Accelerated Anode Degradation in SOFCs

Solid oxide fuel cell (SOFC) applications require lifetimes of several years on the system level. A big challenge is to demonstrate such exceptionally long lifetimes in ongoing R&D projects. Accelerated or compressed testing are alternative methods to obtain this. Activities in this area have been carried out without arriving at a generally accepted methodology. This is mainly due to the complexity of degradation mechanisms on the single SOFC components as function of operating parameters. In this study, we present a detailed analysis of approx. 180 durability tests regarding degradation of single SOFC components as function of operating conditions. Electrochemical impedance data were collected on the fresh and long-term tested SOFCs and used to de-convolute the individual losses of single SOFC cell components – electrolyte, cathode and anode. The main findings include a time-dependent effect on degradation rates and the domination of anode degradation for the evaluated cell types and operating conditions. Specifically, the steam content as determined by fuel inlet composition, current density and fuel utilization was identified as major parameter, more important than for example operating temperature. The obtained knowledge is adopted to identify optimal operation profiles in order to acquire accelerated testing for lifetime investigation of SOFCs.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry
Authors: Ploner, A. (Intern), Hagen, A. (Intern), Hauch, A. (Intern)
Pages: 498-507
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Fuel Cells
Volume: 17
Issue number: 4
ISSN (Print): 1615-6846
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 1.88 SJR 0.559 SNIP 0.748
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.79 SJR 0.495 SNIP 0.603
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.685 SNIP 0.779 CiteScore 2.02
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.615 SNIP 0.792 CiteScore 2.05
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.835 SNIP 0.833 CiteScore 1.99
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.24 SNIP 0.993 CiteScore 2.76
ISI indexed (2012): ISI indexed yes
Subsolidus Phase Relations of the CoO\textsubscript{x}-CuO-SrO System

The subsolidus phase relations of the CoO\textsubscript{x}-CuO-SrO system were investigated in air. The samples were equilibrated at 900 °C. The pseudo-ternary section contains three stoichiometric binary oxide phases (Sr\textsubscript{2}CuO\textsubscript{3}, SrCuO\textsubscript{2} and Sr\textsubscript{14}Cu\textsubscript{24}O\textsubscript{41−δ}) and a binary oxide solid solution: Sr\textsubscript{6+x}Co\textsubscript{5}O\textsubscript{15+δ} (0 ≤ x ≤ 0.36). Two binary phases extend into the ternary system forming solid solutions, i.e., Sr\textsubscript{14}Cu\textsubscript{24−x}Co\textsubscript{x}O\textsubscript{41−δ} (0 ≤ x ≤ 5) and Sr\textsubscript{6+x}Co\textsubscript{5−y}Cu\textsubscript{y}O\textsubscript{15+δ} (0 ≤ x ≤ 0.36, 0 ≤ y ≤ 1.0). The Sr\textsubscript{6+x}Co\textsubscript{5}O\textsubscript{15+δ} solid solution was found to undergo a phase separation into a mixture of Sr\textsubscript{6}Co\textsubscript{5}O\textsubscript{15−δ} and Sr\textsubscript{14}Co\textsubscript{11}O\textsubscript{33} upon annealing at 600 °C. This transformation is reversible.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Authors: Grivel, J. (Intern)
Pages: 646-655
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Phase Equilibria and Diffusion
Volume: 38
Issue number: 5
ISSN (Print): 1547-7037
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 1.12 SJR 0.575 SNIP 0.864
SUN HUB – ENERGY HUB FOR OUTDOOR TABLES

Solar cells integrated into products are attracting more and more attention especially due to the dramatically declining cost of solar cells. Furthermore, we are getting more dependent on portable units like mobile phones, tablets and PCs which has to be charged to be of any use. Especially on festivals where people camps for several days it can be hard to have your portable units charged. In this this work we report a solar powered hub, as an add-on to a table in the urban environment for charging mobile phones and tablets and other handheld devices through USBs, charging laptops through AC connections, providing opportunity to stream music via Bluetooth and play it from a handheld device to the table and lastly to provide LED lighting on the table during the dark hours. 3 prototypes of the system was built and tested at the Roskilde Festival 2017. Electrical logger units were built into the 3 Sun Hubs to monitor the overall energy system and the consumption of each functionality in the table.

General information
Suppressed carrier density for the patterned high mobility two-dimensional electron gas at γ-Al2O3/SrTiO3 heterointerfaces

The two-dimensional electron gas (2DEG) at the non-isoostructural interface between spinel γ-Al2O3 and perovskite SrTiO3 is featured by a record electron mobility among complex oxide interfaces in addition to a high carrier density up to the order of 10^{15} cm^{-2}. Herein, we report on the patterning of 2DEG at the γ-Al2O3/SrTiO3 interface grown at 650 °C by pulsed laser deposition using a hard mask of LaMnO3. The patterned 2DEG exhibits a critical thickness of 2 unit cells γ-Al2O3 for the occurrence of interface conductivity, similar to the unpatterned sample. However, its maximum carrier density is found to be approximately 3×10^{13} cm^{-2}, much lower than that of the unpatterned sample (~10^{15} cm^{-2}). Remarkably, a high electron mobility of approximately 3,600 cm^2V^{-1}s^{-1} was obtained at low temperatures for the patterned 2DEG at a carrier density of ~7×10^{12} cm^{-2}, which exhibits clear Shubnikov-de Hass quantum oscillations. The patterned high-mobility 2DEG at the γ-Al2O3/SrTiO3 interface paves the way for the design and application of spinel/perovskite interfaces for high-mobility all-oxide electronic devices.
Surface characterization of coated cathodes with lithium phosphorous oxynitride thin film for all-solid-state Li-S batteries

General information
State: Published
Organisations: Department of Energy Conversion and Storage
Authors: Lefevr, J. (Intern), Blanchard, D. (Intern), Stamate, E. (Intern)
Number of pages: 1
Publication date: 2017
Surface defects on the Gd₂Zr₂O₇ oxide films grown on textured NiW technical substrates by chemical solution method

Epitaxial growth of oxide thin films has attracted much interest because of their broad applications in various fields. In this study, we investigated the microstructure of textured Gd₂Zr₂O₇ films grown on (001) (100) orientated NiW alloy substrates by a chemical solution deposition (CSD) method. The aging effect of precursor solution on defect formation was thoroughly investigated. A slight difference was observed between the as-obtained and aged precursor solutions with respect to the phase purity and global texture of films prepared using these solutions. However, the surface morphologies are different, i.e., some regular-shaped regions (mainly hexagonal or dodecagonal) were observed on the film prepared using the as-obtained precursor, whereas the film prepared using the aged precursor exhibits a homogeneous structure. Electron backscatter diffraction and scanning electron microscopy analyses showed that the Gd₂Zr₂O₇ grains present within the regular-shaped regions are polycrystalline, whereas those present in the surrounding are epitaxial. Some polycrystalline regions ranging from several micrometers to several tens of micrometers grew across the NiW grain boundaries underneath. To understand this phenomenon, the properties of the precursors and corresponding xerogel were studied by Fourier transform infrared spectroscopy and coupled thermogravimetry/differential thermal analysis. The results showed that both the solutions mainly contain small Gd[ZrO] clusters obtained by the reaction of zirconium acetylacetonate with propionic acid during the precursor synthesis. The regular-shaped regions were probably formed by large Gd[ZrO] frameworks with a metastable structure in the solution with limited aging time. This study demonstrates the importance of the precise control of chemical reaction path to enhance the stability and homogeneity of the precursors of the CSD route.
Surface-Initiated Atom Transfer Radical Polymerization from Electrospun Mats: An Alternative to Nafion
Proton exchange membranes for fuel cell applications are synthesized by surface-initiated (SI) atom transfer radical polymerization (ATRP). Poly(vinylidene fluoride-co-chlorotrifluoroethylene) is electrospun into 50 μm thick mat, which is then employed as multifunctional initiator for copper-mediated SI ATRP of 4-styrene sulfonic acid sodium salt. Fine-tuning of the ATRP conditions allows adjustment of the membrane's ion exchange capacity by varying the loading of the grafted ionomer. Structure and composition of the membranes are investigated by spectroscopic means and thermogravimetric analysis, respectively. The membrane morphology is probed by scanning electron microscopy. A membrane with proton conductivity as high as 100 mS cm⁻¹ is obtained. Long-term durability study in direct methanol fuel cells is conducted for over 1500 h demonstrating the viability of this novel facile approach.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, The Danish Polymer Centre, Department of Energy Conversion and Storage, Bulgarian Academy of Sciences, Teknologisk Institut
Authors: Javakhishvili, I. (Intern), Dimitrov, I. (Ekstern), Tynelius, O. (Ekstern), Hales, J. H. (Ekstern), Jankova Atanasova, K. (Intern), Hvilsted, S. (Intern)
Publication date: 2017
Main Research Area: Technical/natural sciences
Sustainable future alternatives to petroleum-based polymeric conservation materials

The research described here is the first study on the use of sustainable, plant-based biopolymers in conservation practice. Two applications of biopolymers to conservation were investigated – in commercial bioplastics as substitutes for petroleum-based plastic packaging, and in novel adhesive and coating formulations. Bio-polyethylenes, bio-polyesters and
bio-cellulose-based products were evaluated against petroleum-based materials. Bio- and petroleum-based polyethylenes shared optical, chemical and thermal properties. Bamboo and sugarcane fibre containers were also chemically stable. Polyester polylactic acid (PLA) bags and containers became brittle and opaque at a relative humidity (RH) above 65%. FTIR spectroscopy and thermogravimetric analysis suggested that PLA hydrolysed to produce acids. PLA/cornstarch bags fragmented on ageing and formed a gel at high RH levels. A 5 wt% solution of adhesive prepared from soya protein was an effective and reversible adhesive for wood, paper and glass, but adhered poorly to polyethylene and poly(methyl methacrylate). Humic acid-based solutions formed cohesive films which adhered well to glass, paper and soil.

**General information**

State: Published
Organisations: Department of Energy Conversion and Storage, The National Museum of Denmark, ICA Art Conservation
Authors: Shashoua, Y. (Ekstern), Jankova Atanasova, K. (Intern), Curran, C. (Ekstern)
Number of pages: 3
Publication date: 2017

**Host publication information**

Title of host publication: ICOM-CC 18th Triennial Conference Preprints, Copenhagen, 4–8 September 2017,
Place of publication: Paris
Publisher: International Council of Museums
Editor: J. B.
Article number: 1610
Main Research Area: Technical/natural sciences
Conference: 18th Triennial Conference, Copenhagen, Denmark, 04/09/2017 - 04/09/2017
Sustainable, Biopolymer, Bioplastic polyethylene, Polyester, Soya, Humic Acid
Source: Findit
Source-ID: 2396791786
Publication: Research › Article in proceedings – Annual report year: 2018

**Synthesis of conjugated polymers with complex architecture for photovoltaic applications**

A common approach to bulk heterojunction solar cells involves a “trial-and-error” approach in finding optimal kinetically unstable morphologies. An alternative approach assumes the utilization of complex polymer architectures, such as donor–acceptor block copolymers. Because of a covalent preorganization of the donor and acceptor components, these materials may form desirable morphologies at thermodynamic equilibrium. This chapter reviews synthetic approaches to such architectures and shows the first photovoltaic results.

**General information**

State: Published
Organisations: Department of Energy Conversion and Storage, Organic Energy Materials, Leibniz-Institut für Polymerforschung Dresden e.V.
Authors: Kiriy, A. (Ekstern), Krebs, F. C. (Intern)
Number of pages: 26
Pages: 351-376
Publication date: 2017

**Host publication information**

Title of host publication: Elementary Processes in Organic Photovoltaics
Publisher: Springer
ISBN (Print): 978-3-319-28336-4
ISBN (Electronic): 978-3-319-28338-8
Series: Advances in Polymer Science
Volume: 272
ISSN: 0065-3195
Main Research Area: Technical/natural sciences
Chemical Engineering (all), Polymers and Plastics, Organic Chemistry, Catalyst-transfer polycondensation, Covalent preorganization, Donor-acceptor block copolymer, Grafting-from, Grafting-through, Grafting-to, Hairy particles, Morphology, PCBM, Self-assembly, Suzuki chain-growth polycondensation
DOI: 10.1007/978-3-319-28338-8_15
Source: Findit
Source-ID: 2350930220
Publication: Research - peer-review › Book chapter – Annual report year: 2017

**Testing of Electrodes, Cells and Short Stacks**

The present contribution describes the electrochemical testing and characterization of electrodes, cells, and short stacks. To achieve the maximum insight and results from testing of electrodes and cells, it is obviously necessary to have a good
understanding of the fundamental principles of electrochemistry, but it also requires proper test geometries and set up, well-chosen operating conditions for different test purposes, correct probing of voltages and temperatures, and solid knowledge on benefits and drawbacks of different characterization techniques to obtain reliable, accurate, and reproducible electrochemical measurements, and this will be the focus of this chapter. First, the important issue of understanding potential differences and measurements of potentials, which is linked to the choice of proper electrode geometries and test set up configurations for electrode and cell testing, is presented. Then probing of voltages and temperatures, choice of sealing and contacting, as well as considerations regarding the choice of operating conditions for different purposes mainly for single cell testing are outlined. Having considered optimization of test set up, geometries, and the selection of optimal operating conditions, the details of measurement of the electrochemical performance of the electrode, cell, or stack are explained. As part of this, the concept of area specific resistance (ASR) and how DC and AC methods can be used and optimized to provide not only the total ASR, but also the electrochemical characterization of specific parts (electrolyte, each electrode) in a full cell are described. Some experimental results are provided including illustrative examples of breakdown of losses in full cells and determination of their temperature and gas composition dependencies, and finally, challenging issues, such as the effects of impurities and the problem of leakage in cell testing, are discussed as well.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry, Fundamental Electrochemistry
Authors: Hauch, A. (Intern), Mogensen, M. B. (Intern)
Pages: 31-76
Publication date: 2017

The Atomic Simulation Environment - A Python library for working with atoms
The Atomic Simulation Environment (ASE) is a software package written in the Python programming language with the aim of setting up, steering, and analyzing atomistic simulations. In ASE, tasks are fully scripted in Python. The powerful syntax of Python combined with the NumPy array library make it possible to perform very complex simulation tasks. For example, a sequence of calculations may be performed with the use of a simple "for-loop" construction. Calculations of energy, forces, stresses and other quantities are performed through interfaces to many external electronic structure codes or force fields using a uniform interface. On top of this calculator interface, ASE provides modules for performing many standard simulation tasks such as structure optimization, molecular dynamics, handling of constraints and performing nudged elastic band calculations.

General information
State: Published
Organisations: Department of Physics, Theoretical Atomic-scale Physics, Department of Energy Conversion and Storage, Atomic scale modelling and materials, Department of Micro- and Nanotechnology, Theoretical Nanotechnology, Universitat de Barcelona, University of Copenhagen, Malmö University, SINTEF, Aarhus University, Brown University, University of Wisconsin-Madison, University of Warwick, Carnegie Mellon University, Purdue University, Siminn, Karlsruhe Institute of Technology KIT, ETH Zurich, University of Freiburg
Number of pages: 30
Publication date: 2017
The Effect of Electrical Polarization on Electronic Structure in LSM Electrodes: An Operando XAS, RIXS and XES Study

The influence of electrical polarization on Mn in La$_{0.5}$Sr$_{0.5}$MnO$_{3}$ electrodes has been investigated by operando High Energy Resolved Fluorescence Detected X-Ray Absorption Near-Edge Structure (HERFD-XANES) spectroscopy, K$_\beta$ X-ray Emission Spectroscopy (XES) and Resonant Inelastic X-ray Scattering (RIXS) at the Mn K-edge. The study of polarization induced changes in the electronic properties and structure has been carried out at 500°C in 10–20% O$_2$ with electrical polarization applied in the range from −850 mV to 800 mV. Cathodic polarizations in the range −600 mV to −850 mV induced a shift in the Mn K edge energy towards lower energies. The shift is assigned to a decrease in the average Mn oxidation state, which based on K$_\beta$ XES changes from 3.4 at open circuit voltage to 3.2 at −800 mV applied potential. Furthermore, RIXS rendered pronounced changes in the population of the Mn 3d orbitals, due to filling of the Mn d-orbitals during the cathodic polarization. Overall, the study experimentally links the electrical polarization of LSM electrodes to the structural and electronic properties of Mn - these properties are expected to be of major importance for the electrocatalytic performance of LSM electrode towards the oxygen reduction reaction.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Karlsruhe Institute of Technology KIT
Authors: Traulsen, M. L. (Intern), Carvalho, H. (Ekstern), Zielke, P. (Intern), Grunwaldt, J. (Ekstern)
Pages: F3064-F3072
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of The Electrochemical Society
Volume: 164
Issue number: 10
ISSN (Print): 0013-4651
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 3.48 SJR 1.267 SNIP 1.009
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.97 SJR 1.222 SNIP 0.963
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.115 SNIP 1.066 CiteScore 3.17
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.213 SNIP 1.25 CiteScore 3.36
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.169 SNIP 1.309 CiteScore 2.92
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
The Effect of Nano-TiC Addition on Sintered Nd-Fe-B Permanent Magnets

This paper addresses the effect of nano-TiC addition on sintered Nd-Fe-B permanent magnets. TiC nanoparticles were added to sintered Nd-Fe-B magnets with a specific aim to improve the Curie temperature and thermal stability. A standard powder metallurgy route was adopted to prepare the magnets. It was found that introducing nano-TiC prior to jet milling was effective as the nanoparticles dispersed in the final alloy, concentncalcrating in the neodymium-rich phase of the magnets. Magnets with optimal properties were obtained with the addition of 1 wt% TiC nanoparticles. The hysteresis loop for such magnets showed an improved shape and VSM analysis a coercivity value of 1188 kA/m, a remanence value of 0.96 T and a maximum energy product of 132 kJ/m³. The maximum working point and the Curie temperature of the developed magnets were 373 K and 623 K respectively.
The effect of tapering on a magnetocaloric regenerator bed

To design a high efficiency magnetocaloric heat pump for the residential sector, we focused on the improvement of the performance of the regenerator bed. In particular, placing the regenerators circumferentially on a plane, we decided to use tapered regenerators instead of the straight channel ones. Therefore, this paper investigates the effect of the tapering of the regenerators, which exhibit better air-gap utilization. Several simulations using a 1D AMR model were run to study the performance of the tapered regenerator, and the results were compared to the case of the straight regenerator bed. Moreover, the temperature span was held fixed at 25 K, and the working temperature of the regenerator was shifted to study the sensitivity to the variation of the working conditions. This paper considers a 10-layer regenerator, with Curie temperature (T_C) spacing of 2.5 K.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Authors: Dallolio, S. (Intern), Lei, T. (Intern), Engelbrecht, K. (Intern), Bahl, C. (Intern)
Pages: 300-308
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: International Journal of Refrigeration
Volume: 84
ISSN (Print): 0140-7007
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 1.888 SJR 1.471 CiteScore 3.46
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.06 SJR 1.371 SNIP 1.607
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.349 SNIP 1.532 CiteScore 2.44
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.619 SNIP 2.086 CiteScore 2.6
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.422 SNIP 1.944 CiteScore 2.25
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
The future of transportation in sustainable energy systems: Opportunities and barriers in a clean energy transition

Energy demand of a transport sector has constantly been increasing in the recent years, consuming one third of the total final energy demand in the European Union (EU) over the last decade. A transition of this sector towards sustainable one is facing many challenges in terms of suitable technology and energy resources. Especially challenging transition is envisaged for heavy-weight, long-range vehicles and airplanes. A detailed literature review was carried out in order to detect the current state of the research on clean transport sector, as well as to point out the gaps in the research. In order to calculate the resources needed for the transition towards completely renewable transport sector, four main alternatives to the current fossil fuel systems were assessed and their potential was quantified, i.e. biofuels, hydrogen, synthetic fuels (electrofuels) and electricity. Results showed that electric modes of transport have the largest benefits and should be the main aim of the transport transition. It was calculated that 72.3% of the transport energy demand on the EU level could be directly electrified by the technology existing today. For the remaining part of the transport sector a significant demand for energy resources exists, i.e. 3069 TWh of additional biomass was needed in the case of biofuels utilization scenario while 2775 TWh of electricity and 925 TWh of heat were needed in the case of renewable electrofuels produced using solid oxide electrolysis scenario.
The influence of carbon and oxygen on the magnetic characteristics of press-less sintered NdFeB magnets

The Pressless Process (PLP) was adopted to manufacture NdFeB sintered magnets, where the investigations on carbon and oxygen residues from heptane milling liquid media and graphite crucibles used for sintering were quantified to evaluate the influence on the magnetic characteristics. The carbon and oxygen content in the magnets produced from wet ball milling of strip cast flakes was found to be of the order 104 ppm and 4·104 ppm respectively, which resulted in soft magnetic behavior. However using jet milling the carbon and oxygen concentration were decreased by an order of magnitude resulting in coercivity of up to 829 kA/m. Thus the influence of the carbon from the graphite crucibles is small.

General information
State: Published
Authors: Xia, M. (Intern), Abrahamsen, A. B. (Intern), Bahl, C. (Intern), Veluri, B. (Ekstern), Søegaard, A. I. (Ekstern), Bøjsøe, P. (Ekstern), Millot, S. (Ekstern)
Number of pages: 5
Pages: 232-236
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Magnetism and Magnetic Materials
Volume: 422
ISSN (Print): 0304-8853
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SJR 0.786 SNIP 1.349 CiteScore 2.97
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.41 SJR 0.699 SNIP 1.181
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.73 SNIP 1.296 CiteScore 2.33
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.815 SNIP 1.423 CiteScore 2.07
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.801 SNIP 1.385 CiteScore 2.03
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.928 SNIP 1.294 CiteScore 1.95
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.07 SNIP 1.275 CiteScore 1.84
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.936 SNIP 0.987
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.844 SNIP 0.908
Web of Science (2009): Indexed yes
The La(Fe,Mn,Si)$_{13}$Hz magnetic phase transition under pressure (Phys. Status Solidi RRL 8/2017)

A promising solid-state refrigeration technology, known as magnetic refrigeration, has reached a groundbreaking result. The potential for environmentally friendly cooling using the magnetocaloric effect is disadvantaged by small temperature windows of effective cooling and the requirement of expensive, high magnetic field producing Nd-Fe-B permanent magnets. Researchers from Imperial College London, Ames Laboratory (USA) and DTU Energy, Technical University of Denmark (see article no. 1700143) show through utilising a larger portion of the phase diagram of so-called soft first order magnetic materials that they can reduce the maximum field required to within that attainable with cheap ferrite-based permanent magnets (around 0.5 T) and significantly broaden the working temperature range. Traditionally, magnetocaloric materials are controlled through temperature and applied magnetic field, but with the addition of applied hydrostatic pressure it is possible to move around in the phase diagram of the La(Fe,Mn,Si)$_{13}$Hz material series, taking advantage of its so-called multicaloric properties. By careful choice of magnetic field and pressure controlled cooling cycles this work shows that a significant bottleneck towards commercially competitive refrigeration devices based on the magnetocaloric effect can be overcome.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Administration, Imperial College London, Iowa State University
Authors: Lovell, E. (Ekstern), Bez, H. N. (Ekstern), Boldrin, D. C. (Ekstern), Nielsen, K. K. (Intern), Smith, A. (Intern), Bahl, C. R. H. (Intern), Cohen, L. F. (Ekstern)
Number of pages: 1
Publication date: 2017

Publication information
Original language: English
Volume: 11
Publisher: Wiley-VCH
Main Research Area: Technical/natural sciences
Electronic versions:
DOIs:
10.1002/pssr.201770340
The La(Fe,Mn,Si)$_{13}$H$_{1.65}$ magnetic phase transition under pressure

We study the magnetocaloric metamagnetic transition in LaFe$_{11.74}$Mn$_{0.06}$Si$_{1.20}$ and LaFe$_{11.76}$Mn$_{0.06}$Si$_{1.18}$H$_{1.65}$ under hydrostatic pressure up to 1.2 GPa. For both compounds, hydrostatic pressure depresses the zero field critical temperature. However, in detail, pressure influences the magnetic properties in different ways in the two compounds. In the dehydrogenated case the transition broadens under pressure whereas in the hydrogenated case the transition sharpens. In both cases thermal hysteresis increases under pressure, although with different trends. These observations suggest both intrinsic and extrinsic hysteresis loss brought about by the use of hydrostatic pressure. We explore the multicaloric field-pressure cycle, demonstrating that although the gain introduced by overcoming the magnetic hysteresis loss is closely countered by the loss introduced in the pressure cycle, there are significant advantages in that the temperature range of operation can be finely tuned and extended, and the magnetocaloric transition can operate in lower absolute applied fields (<0.5 T), potentially overcoming one of the most significant bottlenecks to the commercialization of this technology.
The maximum theoretical performance of unconcentrated solar photovoltaic and thermoelectric generator systems

The maximum efficiency for photovoltaic (PV) and thermoelectric generator (TEG) systems without concentration is investigated. Both a combined system where the TEG is mounted directly on the back of the PV and a tandem system where the incoming sunlight is split, and the short wavelength radiation is sent to the PV and the long wavelength to the TEG, are considered. An analytical model based on the Shockley-Queisser efficiency limit for PVs and the TEG figure of merit parameter $zT$ is presented. It is shown that for non-concentrated sunlight, even if the TEG operates at the Carnot efficiency and the PV performance is assumed independent of temperature, the maximum increase in efficiency is 4.5 percentage points (pp.) for the combined case and 1.8 pp. for the tandem case compared to a stand alone PV. For a more realistic case with a temperature dependent PV and a realistic TEG, the gain in performance is much lower. For the combined PV and TEG system it is shown that a minimum $zT$ value is needed in order for the system to be more efficient than a stand alone PV system.
The promise of negative emissions

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry, Livermore, Arizona State University, Columbia University, University of California, Colorado School of Mines
Authors: Lackner, K. S. (Ekstern), Aines, R. (Ekstern), Atkins, S. (Ekstern), Barrett, S. (Ekstern), Barteau, M. (Ekstern), Braun, R. J. (Ekstern), Brouwer, J. (Ekstern), Broecker, W. (Ekstern), Browne, J. B. (Ekstern), Graves, C. R. (Intern)
Pages: 714
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Science
Volume: 354
Issue number: 6313
ISSN (Print): 0036-8075
Ratings:
BFI (2018): BFI-level 3
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 15.85 SJR 14.142 SNIP 7.154
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 14.39 SJR 13.745 SNIP 7.547
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 12.052 SNIP 8.129 CiteScore 12.68
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 12.41 SNIP 7.809 CiteScore 12.43
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 14.238 SNIP 8.277 CiteScore 11.97
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 13.481 SNIP 7.773
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 11.897 SNIP 7.056
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 11.277 SNIP 6.075
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 10.072 SNIP 6.017
Web of Science (2007): Indexed yes
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 11.09 SNIP 6.563
Web of Science (2005): Indexed yes
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 11.428 SNIP 7.488
Web of Science (2003): Indexed yes
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 10.987 SNIP 6.94
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 15.245 SNIP 7.042
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 16.615 SNIP 7.018
Original language: English
DOIs:
10.1126/science.aal2432

Bibliographical note
The full list of 46 authors and affiliations is available in the supplementary materials.
Source: PublicationPreSubmission
Source-ID: 128838973
Thermal behavior and decomposition of cerium(III) butanoate, pentanoate and hexanoate salts upon heating in argon

The thermal behavior and decomposition of Ce-butanoate monohydrate (Ce(C₃H₇CO₂)₃·H₂O), Ce-pentanoate (Ce(C₄H₉CO₂)₃) and Ce-hexanoate (Ce(C₅H₁₁CO₂)₃) were studied in a flow of argon while heating at 5 °C/min. By means of several techniques such as simultaneous TG-DTA, FTIR evolved gas analysis, in-situ x-ray diffraction using a synchrotron source and hot-stage microscopy, it was found that all three compounds undergo melting transitions prior to decomposition and that decomposition involves intermediate stages including at least a Ce₂O(CnH₂n+1CO₂)₄ intermediate (n = 3, 4 or 5 for Ce-butanoate, pentanoate or hexanoate respectively). The final decomposition product consists of CeO₂, which is formed through a Ce-oxycarbonate. The Ce³⁺ → Ce⁴⁺ oxidation seems to proceed via Ce₂O₃ that first results from the decomposition of the oxycarbonate phase. During the whole decomposition process, the evolved gas species consist of CO₂ and symmetrical ketones.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Deutsches Elektronen-Synchrotron
Authors: Grivel, J. (Intern), Suarez Guevara, M. J. (Intern), Yue, Z. (Intern), Tang, X. (Intern), Pallewatta, P. G. A. P. (Intern), Bednarcik, J. (Ekstern)
Pages: 77-87
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Analytical and Applied Pyrolysis
Volume: 126
ISSN (Print): 0165-2370
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 1.312 SJR 1.129 CiteScore 3.91
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.11 SJR 1.379 SNIP 1.572
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.489 SNIP 1.635 CiteScore 4.06
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.691 SNIP 1.954 CiteScore 4.08
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.036 SNIP 1.921 CiteScore 3.6
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.408 SNIP 1.77 CiteScore 3.26
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.388 SNIP 1.603 CiteScore 3.07
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.181 SNIP 1.424
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.296 SNIP 1.418
BFI (2008): BFI-level 1
The thermal operating window for PEDOT:PSS films and its related thermoelectric properties

The intrinsically conducting polymer PEDOT:PSS is widely used and has found high recognition due to its excellent electrical conductivity. Its potential applications cover many fields, e.g. thermoelectric energy conversion. Therefore we compared the thermoelectric properties of pristine and DMSO treated PEDOT:PSS films at potential operating temperatures. Here we observed the electrical degradation of the film up to complete failure. Further, the thermal aging of PEDOT:PSS still lacks of understanding. It is pointed out that PEDOT:PSS films show a complex degradation mechanism which includes a morphological and a chemical part. In the range of room temperature and ~160 °C PEDOT:PSS films follow the known exponential degradation which imposes morphological degradation, while at higher temperatures this law is not suitable to match the experimental data. Thus we extended the known exponential equation by an additional exponential degradation term which shows good agreement with the experimental data. The optical absorption spectrum indicates a loss in bipolaron and polaron charge carriers, which reflects the degradation behavior. It can be seen that changes in the optical absorption spectrum after isothermal annealing for more than 50 h occur at temperatures around 120 °C, which marks the transition from morphological to chemical degradation.

General information

State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Ceramic Engineering & Science, Fraunhofer Institute for Material and Beam Technology
Authors: Stepień, L. (Ekstern), Roch, A. (Ekstern), Tkachov, R. (Ekstern), Leupolt, B. (Ekstern), Han, L. (Intern), Van Nong, N. (Intern), Leyens, C. (Ekstern)
Pages: 49-54
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information

Journal: Synthetic Metals
Volume: 225
ISSN (Print): 0379-6779
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 0.766 SJR 0.672 CiteScore 2.49
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.666 SNIP 0.756 CiteScore 2.45
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.624 SNIP 0.735 CiteScore 2.27
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.709 SNIP 0.934 CiteScore 2.42
Web of Science (2014): Indexed yes
Thermodynamic assessment of the oxygen reduction activity in aqueous solutions

In the conventional theoretical approach, oxygen reduction reaction activities are assessed through a volcano plot using activity descriptors. The volcano plot relies on several approximations, e.g. the reaction kinetics are commonly overlooked and the interaction of hydrophilic intermediates with water is considered constant regardless of the metal surface. Herein, we demonstrate by means of density functional theory calculations that the binding energies of hydrophilic intermediates are strongly influenced by hydrogen bonding (HB) to surface water molecules. We find the HB energies of adsorbed OOH and OH on a number of active metallic (strained and non-strained Pt, Pd, Ag) and bimetallic (Pt3Ni, Pt3Co, PtCu, Pd@Pt-skin and Pt@Pd-skin) 111 surfaces to vary by up to 0.5 eV in energy. Furthermore, we show that the existence of a universal scaling line is a relative notion, contingent on how large errors in activity predictions can be tolerated. Scaling errors can be reduced substantially by partitioning data into subsets depending on the element comprising the surface layer. Finally, the activity volcano that explicitly includes HB and van der Waals interactions reproduces the right experimental trend for Pt and its alloys, but at the same time predicts Ag to be a more active catalyst than Pt. The latter result can be explained by having a fundamentally different water structure on Ag(111) than on the other metals, and the fact that reaction kinetics have been neglected in the analysis.

General information

State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials
Thermodynamic Ground States of Complex Oxide Heterointerfaces

The formation mechanism of 2-dimensional electron gases (2DEGs) at heterointerfaces between nominally insulating oxides is addressed with a thermodynamical approach. We provide a comprehensive analysis of the thermodynamic ground states of various 2DEG systems directly probed in high temperature equilibrium conductivity measurements. We unambiguously identify two distinct classes of oxide heterostructures: For epitaxial perovskite/perovskite heterointerfaces (LaAlO3/SrTiO3, NdGaO3/SrTiO3, and (La,Sr)(Al,Ta)O3/SrTiO3), we find the 2DEG formation being based on charge transfer into the interface, stabilized by the electric field in the space charge region. In contrast, for amorphous LaAlO3/SrTiO3 and epitaxial γ-Al2O3/SrTiO3 heterostructures, the 2DEG formation mainly relies on the formation and accumulation of oxygen vacancies. This class of 2DEG structures exhibits an unstable interface reconstruction associated with a quenched nonequilibrium state.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, RWTH Aachen University, Forschungszentrum Jülich GmbH
Authors: Gunkel, F. (Ekstern), Hoffmann-Eifert, S. (Ekstern), Heinen, R. A. (Ekstern), Christensen, D. V. (Intern), Chen, Y. (Intern), Pryds, N. (Intern), Waser, R. (Ekstern), Dittmann, R. (Ekstern)
Number of pages: 7
Pages: 1086–1092
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: A C S Applied Materials and Interfaces
Volume: 9
Issue number: 1
ISSN (Print): 1944-8244
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 8.15 SJR 2.784 SNIP 1.543
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 7.6 SJR 2.561 SNIP 1.536
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 2.262 SNIP 1.555 CiteScore 7.38
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.125 SNIP 1.636 CiteScore 6.88
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.992 SNIP 1.548 CiteScore 6.05
Thermofluid topology optimization of heat sinks

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Department of Mechanical Engineering, Solid Mechanics
Authors: Haertel, J. H. K. (Intern), Lei, T. (Intern), Alexandersen, J. (Intern), Engelbrecht, K. (Intern), Lazarov, B. S. (Intern), Sigmund, O. (Intern)
Number of pages: 1
Publication date: 2017
Event: Poster session presented at Danish Days on Caloric Materials and Devices, Roskilde, Denmark.
Main Research Area: Technical/natural sciences
Electronic versions:
Poster_Haertel_et_al_2017.pdf
Publication: Research › Poster – Annual report year: 2017

Thermoneutral Operation of Solid Oxide Electrolysis Cells in Potentiostatic Mode

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Applied Electrochemistry
Authors: Chen, M. (Intern), Sun, X. (Intern), Chatzichristodoulou, C. (Intern), Koch, S. (Intern), Hendriksen, P. V. (Intern), Mogensen, M. B. (Intern)
Number of pages: 1
Publication date: 2017

Host publication information
Title of host publication: ECS Meeting Abstracts
Volume: MA2017-03
Publisher: The Electrochemical Society
Article number: 287
Main Research Area: Technical/natural sciences
Conference: 15th International Symposium on Solid Oxide Fuel Cells (SOFC-XV), Hollywood, United States, 23/07/2017 - 23/07/2017
Links:
http://ma.ecsdl.org.proxy.findit.dtu.dk/content/MA2017-03/1/287
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2017
Thermoneutral Operation of Solid Oxide Electrolysis Cells in Potentiostatic Mode

High temperature electrolysis based on solid oxide electrolysis cells (SOECs) is a promising technology for energy storage and synthetic fuel production. In recent years extensive efforts have been devoted to improving performance and durability of SOEC cells and stacks. Due to historical reasons and the convenience of doing constant current tests, (almost) all the reported SOEC tests have been galvanostatic. In this work, we report test results on two types of SOEC cells operated for electrolysis of steam in potentiostatic mode at 1.29 V. Both cells are Ni/YSZ fuel electrode supported type with different oxygen electrodes. The two cells exhibited different initial performance and different long-term degradation behavior. Detailed impedance analysis indicates that degradation happened mainly at the Ni/YSZ electrode for both cells. Large overpotential on the Ni/YSZ electrode was identified as the main cause of the degradation. Operation strategies were further proposed for electrolysis operation in potentiostatic mode.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Applied Electrochemistry
Authors: Chen, M. (Intern), Sun, X. (Intern), Chatzichristodoulou, C. (Intern), Koch, S. (Intern), Hendriksen, P. V. (Intern), Mogensen, M. B. (Intern)
Pages: 3077-3088
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: E C S Transactions
Volume: 78
Issue number: 1
ISSN (Print): 1938-5862
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 0.44 SJR 0.225 SNIP 0.252
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 0.4 SJR 0.228 SNIP 0.253
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.211 SNIP 0.244 CiteScore 0.36
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.212 SNIP 0.234 CiteScore 0.36
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.192 SNIP 0.231 CiteScore 0.27
ISI indexed (2013): ISI indexed no
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.241 SNIP 0.26 CiteScore 0.29
ISI indexed (2012): ISI indexed no
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.261 SNIP 0.28 CiteScore 0.36
ISI indexed (2011): ISI indexed no
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.249 SNIP 0.251
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.242 SNIP 0.27
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.254 SNIP 0.255
Scopus rating (2007): SJR 0.213 SNIP 0.206
Scopus rating (2006): SJR 0.134 SNIP 0.073
Original language: English
Electronic versions:
Paper_101149_manuscript_21611_0.pdf
DOIs:
10.1149/07801.3077ecst
Publication: Research - peer-review › Journal article – Annual report year: 2017
The role of CO* as a spectator in CO₂ electro-reduction on RuO₂
RuO₂-based electrocatalysts are found to be active at low overpotential toward direct electrochemical reduction of CO₂ to formic acid and methanol. RuO₂ can circumvent the thermodynamic bottleneck resulting from the scaling relations observed on metallic electrocatalyst, by utilizing an alternate pathway through oxygen-coordinated intermediates. Employing density functional theory based computational electrocatalysis models we show adsorbate–adsorbate interaction effects for adsorbates and reaction intermediates on the RuO₂(110) surface are large and impactful to the reaction thermodynamics. We studied binding energy amendment due to adsorbate interaction (steric and electronic) with varying coverage of CO* spectators on the catalyst surface. Implications on the reaction pathways help us rationalize differences in experimentally observed carbonaceous product mix and suppression of the hydrogen evolution reaction (HER). We show that a moderate CO* coverage (~50%) is necessary for obtaining methanol as a product and that higher CO* coverages leads to very low overpotential for formic acid evolution. Our analysis also clarifies the importance of the reaction condition for CO₂ reduction to liquid fuels utilizing RuO₂-based electrocatalysts.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials
Authors: Bhowmik, A. (Intern), Hansen, H. A. (Intern), Vegge, T. (Intern)
Pages: 18333-18343
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: The Journal of Physical Chemistry Part C
Volume: 121
Issue number: 34
ISSN (Print): 1932-7447
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 4.58 SJR 2.135 SNIP 1.147
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.48 SJR 1.964 SNIP 1.195
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.886 SNIP 1.26 CiteScore 4.68
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.032 SNIP 1.447 CiteScore 5.08
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 2.143 SNIP 1.445 CiteScore 5.14
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.529 SNIP 1.461 CiteScore 4.98
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.339 SNIP 1.465 CiteScore 4.92
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 2.462 SNIP 1.362
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Thickness-Dependent Properties of YBCO Films Grown on GZO/CLO-Buffered NiW Substrates

To study the role of novel Gd$_2$Zr$_2$O$_7$/Ce$_{0.2}$La$_{0.8}$O$_2$ buffer layer structure on a biaxially textured NiW substrate, a set of YBa$_2$Cu$_3$O$_{7-x}$ (YBCO) films with different thicknesses were prepared by pulsed laser deposition (PLD). Interface imperfections as well as thickness-dependent structural properties were observed in the YBCO thin films. The structure is also reflected into the improved superconducting properties with the highest critical current densities in films with intermediate thicknesses. Therefore, it can be concluded that the existing buffer layers need more optimization before they can be successfully used for films with various thicknesses. This issue is linked to the extremely susceptible growth method of PLD when compared to the commonly used chemical deposition methods. Nevertheless, PLD-grown films can give a hint on what to concentrate to be able to further improve the buffer layer structures for future coated conductor technologies.
Three-dimensional graphene anchored Fe$_2$O$_3$@C core-shell nanoparticles as supercapacitor electrodes

Three-dimensional (3D) reduced graphene oxide (rGO) anchored carbon-coated Fe$_2$O$_3$ core-shell nanoparticles (Fe$_2$O$_3$@C-rGO) has been developed successfully through a simple one-pot hydrothermal process followed by a further annealing treatment. The 3D Fe$_2$O$_3$@C-rGO nanocomposite consists of carbon-coated Fe$_2$O$_3$ nanoparticle clusters (Fe$_2$O$_3$@C) and rGO nanosheets. The homogenously distributed and intercalated Fe$_2$O$_3$@C nanoparticles between rGO nanosheets form a highly conductive 3D carbon network with rGO, and present a hierarchical pore size structure, enabling fast ion and electron transport, as well as remarkable specific surface area. The electrochemical performance in supercapacitor has been characterized, and the as-prepared Fe$_2$O$_3$@C-rGO electrode shows a significant high specific capacitance of 211.4 F/g at 0.5 A/g and 177.2 F/g at 20 A/g with no visible performance decay even after 2500 cycles testing. These properties indicate a good potential to achieve high performance electrochemical devices.

General information

State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors, Tianjin University
Authors: Zhang, M. (Ekstern), Sha, J. (Ekstern), Miao, X. (Ekstern), Liu, E. (Ekstern), Shi, C. (Ekstern), Li, J. (Ekstern), He, C. (Ekstern), Li, Q. (Intern), Zhao, N. (Ekstern)
Number of pages: 8
Pages: 956-963
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Alloys and Compounds
Volume: 696
ISSN (Print): 0925-8388
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SJR 1.02 SNIP 1.403 CiteScore 3.66
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.05 SJR 0.954 SNIP 1.332
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.957 SNIP 1.398 CiteScore 3.03
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.117 SNIP 1.632 CiteScore 3.13
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.059 SNIP 1.583 CiteScore 2.73
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.246 SNIP 1.57 CiteScore 2.43
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.164 SNIP 1.463 CiteScore 2.41
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.073 SNIP 1.223
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.956 SNIP 1.372
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.888 SNIP 1.21
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.882 SNIP 1.209
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 0.901 SNIP 1.158
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.088 SNIP 1.208
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.922 SNIP 1.354
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 0.949 SNIP 1.051
Scopus rating (2002): SJR 0.733 SNIP 1.063
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.634 SNIP 0.966
Topology optimization and lattice Boltzmann methods
This thesis demonstrates the application of the lattice Boltzmann method for topology optimization problems. Specifically, the focus is on problems in which time-dependent flow dynamics have significant impact on the performance of the devices to be optimized. The thesis introduces new topology optimization problems for both isothermal and thermal flows, and it is demonstrated that topology optimization can account for unsteady flow effects during the optimization process. The introduced optimization problems are solved using a gradient-based approach, and the design sensitivities are computed using a discrete adjoint approach. To handle the complexity of the discrete adjoint approach more easily, a method for computing it based on automatic differentiation is introduced, which can be adapted to any lattice Boltzmann type method. For example, while it is derived in the context of an isothermal lattice Boltzmann model, it is shown that the method can be easily extended to a thermal model as well.

Finally, the predicted behavior of an optimized design is compared to the equivalent prediction from a commercial finite element solver. It is found that the weakly compressible nature of the lattice Boltzmann method leads to a discrepancy in the predicted outcomes. Further research is required to determine which prediction is more accurate, and what implications the discrepancy has for the optimized designs.
Topology optimized permanent magnet systems

Topology optimization of permanent magnet systems consisting of permanent magnets, high permeability iron and air is presented. An implementation of topology optimization for magnetostatics is discussed and three examples are considered. The Halbach cylinder is topology optimized with iron and an increase of 15% in magnetic efficiency is shown. A topology optimized structure to concentrate a homogeneous field is shown to increase the magnitude of the field by 111%. Finally, a permanent magnet with alternating high and low field regions is topology optimized and a $\Lambda_{cool}$ figure of merit of 0.472 is reached, which is an increase of 100% compared to a previous optimized design.
Toward a drone-based EL and PL inspection tool for PV power plants

On-site inspection of PV systems has been historically performed through visual inspection, infrared (IR) thermography, and electrical measurements. Recent advances and cost reductions in unmanned aerial vehicle (UAV) technology have led to adoption of UAVs equipped with thermal cameras for inspection of PV plants, which survey power plants in a fraction of the time and cost than walk through IR imaging. IR imaging however, is limited only to detection of certain fault types that result in elevated temperatures. Techniques such as electro-(EL) and photo-(PL) luminescence imaging offer a higher level of image detail and qualitative insight compared to IR thermography. Furthermore, detection and identification of incipient or severe faults in PV panels is more straightforward. This project proposes for the first time a fast and accurate automatic drone-based inspection method for large PV plants that combines IR, EL, PL imaging, and visual images (VI), called DronEL. The overarching goal is to correlate these images with known PV failures such as hotspots, cell cracks, and potential induced degradation. The DronEL project is carried out by a number of academic and commercial partners including Denmark’s Technical University (DTU), Aalborg University (AAU), Sky-watch, SiCon and Kenergy.

General information
State: Published
Organisations: Department of Photonics Engineering, Diode Lasers and LED Systems, Department of Energy Conversion and Storage, Organic Energy Materials, Aalborg University
Authors: Riedel, N. (Intern), Benatto, G. A. D. R. (Intern), Thorsteinsson, S. (Intern), Poulsen, P. B. (Intern), Spataru, S. (Ekstern), Sera, D. (Ekstern)
Publication date: 2017

Host publication information
Title of host publication: PV Reliability Workshop
Main Research Area: Technical/natural sciences
Conference: PV Reliability Workshop, Denver, United States, 28/02/2017 - 28/02/2017
Source: FindIt
Source-ID: 2355411147
Publication: Research - peer-review › Article in proceedings – Annual report year: 2017

Towards a stable ion-solvating polymer electrolyte for advanced alkaline water electrolysis

Advanced alkaline water electrolysis using ion-solvating polymer membranes as electrolytes represents a new direction in the field of electrochemical hydrogen production. Polybenzimidazole membranes equilibrated in aqueous KOH combine the mechanical robustness and gas-tightness of a polymer with the conductive properties of an aqueous alkaline salt solution, and are thus of particular interest in this field of research. This work presents a comprehensive study of ternary alkaline polymer electrolyte systems developed around a polybenzimidazole derivative that is structurally tailored towards
improved stability in alkaline environments. The novel electrolytes are extensively characterized with respect to
physicochemical and electrochemical properties and the chemical stability is assessed in 0-50 wt% aqueous KOH for
more than 6 months at 88 degrees C. In water electrolysis tests using porous 3-dimensional electrodes completely free
from noble metals, they show polarization characteristics comparable to those of commercially available separators and
good performance stability over several days.

**General information**
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors, Simon Fraser University
(Ekstern), Jensen, J. O. (Intern)
Pages: 5055-5066
Publication date: 2017
Main Research Area: Technical/natural sciences

**Publication information**
Journal: Journal of Materials Chemistry A
Volume: 5
Issue number: 10
ISSN (Print): 2050-7488
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 9.61 SJR 3.488 SNIP 1.55
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 8.46 SJR 3.075 SNIP 1.479
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 2.62 SNIP 1.643 CiteScore 8.36
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.331 SNIP 1.514 CiteScore 7.27
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
ISI indexed (2013): ISI indexed no
Web of Science (2013): Indexed yes
Original language: English
Electronic versions:
Post_print_Towards_a_stable_ion_solvating_polymer_electrolyte_for_advanced_alkaline_water_electrolysis.pdf. Embargo
ended: 22/02/2018
DOIs:
10.1039/c6ta10680c
Source: FindIt
Source-ID: 2355800539
Publication: Research - peer-review › Journal article – Annual report year: 2017

**Towards High Power Density Metal Supported Solid Oxide Fuel Cell for Mobile Applications**

**General information**
State: Published
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry, Mixed Conductors, Ceramic
Engineering & Science
Authors: Nielsen, J. (Intern), Persson, Å. H. (Intern), Muhl, T. (Intern), Brodersen, K. (Intern)
Number of pages: 1
Publication date: 2017

**Host publication information**
Title of host publication: ECS Meeting Abstracts
Volume: MA2017-03
Towards High Power Density Metal Supported Solid Oxide Fuel Cell for Mobile Applications

For use of metal supported SOFC in mobile applications it is important to reduce the thermal mass to enable fast start up, increase stack power density in terms of weight and volume and reduce costs. In the present study, we report on the effect of reducing the support layer thickness of 313 μm in DTU SoA MS-SOFCs gradually to 108 μm. The support layer thickness decrease in the DTU co-sintering MS-SOFC fabrication route results in an increased densification of the support layer and a slight decrease in performance. To mitigate the performance loss, the introduction of gas channels by puncturing of the green tape casted support layer was explored. In summary, it was successfully demonstrated on stack relevant sized 12 cm x 12 cm MS-SOFCs that the support layer thickness could be significantly reduced and that the cell performance could be significantly increased by the introduction of gas channels.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry, Mixed Conductors, Ceramic Engineering & Science
Authors: Nielsen, J. (Intern), Persson, Å. H. (Intern), Muhl, T. (Intern), Brodersen, K. (Intern)
Pages: 2029-2037
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: E C S Transactions
Volume: 78
Issue number: 1
ISSN (Print): 1938-5862
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 0.44 SJR 0.225 SNIP 0.252
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 0.4 SJR 0.228 SNIP 0.253
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.211 SNIP 0.244 CiteScore 0.36
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.212 SNIP 0.234 CiteScore 0.36
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.192 SNIP 0.231 CiteScore 0.27
ISI indexed (2013): ISI indexed no
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.241 SNIP 0.26 CiteScore 0.29
ISI indexed (2012): ISI indexed no
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.261 SNIP 0.28 CiteScore 0.36
ISI indexed (2011): ISI indexed no
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.249 SNIP 0.251
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.242 SNIP 0.27
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.254 SNIP 0.255
Scopus rating (2007): SJR 0.213 SNIP 0.206
Towards identifying the active sites on RuO$_2$(110) in catalyzing oxygen evolution

While the surface atomic structure of RuO$_2$ has been well studied in ultra high vacuum, much less is known about the interaction between water and RuO$_2$ in aqueous solution. In this work, in situ surface X-ray scattering measurements combined with density functional theory (DFT) were used to determine the surface structural changes on single-crystal RuO$_2$(110) as a function of potential in acidic electrolyte. The redox peaks at 0.7, 1.1 and 1.4 V vs. reversible hydrogen electrode (RHE) could be attributed to surface transitions associated with the successive deprotonation of –H$_2$O on the coordinatively unsaturated Ru sites (CUS) and hydrogen adsorbed to the bridging oxygen sites. At potentials relevant to the oxygen evolution reaction (OER), an –OO species on the Ru CUS sites was detected, which was stabilized by a neighboring –OH group on the Ru CUS or bridge site. Combining potential-dependent surface structures with their energetics from DFT led to a new OER pathway, where the deprotonation of the –OH group used to stabilize –OO was found to be rate-limiting.
Towards long-term stable solid state electrolyzers with infiltrated catalysts

Renewable energy sources like wind and solar are widely considered as the key technologies to cover our growing demands. However, the fluctuating nature of these sources requires a flexible energy system and storage technologies to ensure that energy supply can be covered in a stable and affordable manner. One of the promising solutions is the production of synthetic fuel by solid oxide electrolyzers. Electricity can be converted to gas and further to liquid products during times of electricity production excess. In times of need, these fuels can be converted back to electricity by either conventional power plants or fuel cells.

Key challenges for a successful commercialization of solid oxide electrolyzers are upscale it, reduce cost and improve durability. Therefore, large efforts are allocated to improve cell performance. As a relatively novel method to introduce electro-catalysts into the porous structure of the electrodes, infiltration has shown very efficient. Solid oxide cells with infiltrated electrodes have been reported to show improved performance compared to conventional cells [1].

In this study, the development of infiltration procedures to improve the stability and catalytic performance of the fuel electrode of solid state electrolyzers (SOEC) will be presented. The infiltration process was optimized through choice of surfactants and concentrations of precursor solutions, to ensure easy penetration of the precursor solution into a Ni-YSZ (yttrium stabilized zirconia) composite backbone. The influence of surfactants on the coverage of specific grains with the infiltrated Ce0.8Gd0.2O2-d (CGO) nano-sized catalyst in the composite backbone was also studied. The optimized infiltration process was applied to 5 x 5 cm solid oxide cells.

The cells composed of a thin YSZ electrolyte, a Ni-YSZ fuel electrode and an LSCF-CGO oxygen electrode were tested in steam electrolysis operation under a current load of up to 1.25 A/cm². Under high steam content and high current density, a fast cell degradation (~700 mV/kh) was observed for un-infiltrated cells. The infiltration of a CGO nano-sized catalyst into the Ni-YSZ backbone was observed to reduce the degradation rate to around 117 mV/kh.

Towards solid oxide electrolysis plants in 2020

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Ceramic Engineering & Science, Applied Electrochemistry, Imaging and Structural Analysis
Authors: Ovtar, S. (Intern), Chen, M. (Intern), Brodersen, K. (Intern), Hauch, A. (Intern), Sun, X. (Intern), Bentzen, J. J. (Intern), Hendriksen, P. V. (Intern)
Number of pages: 1
Publication date: 2017
Event: Abstract from 21st International Conference on Solid State Ionics, Padova, Italy.
Main Research Area: Technical/natural sciences
Electronic versions:
SSI_infiltration_Ovtar.pdf
Source: PublicationPreSubmission
Source-ID: 134385065
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2017

Towards solid oxide electrolysis plants in 2020

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Department of Electrical Engineering, Electronics, Haldor Topsoe AS, Aalborg University
Authors: Chen, M. (Intern), Blennow, P. (Ekstern), Mathiesen, B. V. (Ekstern), Zhang, Z. (Intern)
Number of pages: 1
Publication date: 2017
Main Research Area: Technical/natural sciences
**Tracking Solid Oxide Cell Microstructure Evolution by High Resolution 3D Nano-Tomography**

Solid oxide cells (SOCs) offer great prospects for the efficient and reversible conversion of chemical to electrical energy. Therefore, they are expected to play a key role in the renewable energy landscape. However, their limited lifetime under operating conditions hinders their widespread usage. The degradation processes are mainly attributed to morphological changes occurring within the electrodes microstructure. Therefore, precise tracking of 3D microstructural evolution during operation is considered crucial to understanding the complex relationship between microstructure and performance.

In this work, X-ray ptychographic tomography is applied to SOC materials, demonstrating unprecedented spatial resolution and data quality. The effect of a complete redox cycle on the same Ni-YSZ microstructure is visualized ex-situ in 3D, showing major rearrangement of the nickel network after reduction, the formation of cracks in the YSZ, and void formation in nickel oxide after oxidation.

Capitalizing on the high resolution of ptychography, the effect of nickel coarsening on the Ni-YSZ microstructure evolution is studied ex-situ in three dimensions, while the sample is repeatedly scanned and treated at high temperature in dry hydrogen. The analyses show the substantial evolution of the nickel and pore networks during the first 3 hours of treatment. The nickel coarsening leads to loss of nickel connectivity, a decrease in specific interface area and a decrease in total triple phase boundary density.

The ex-situ experiment on a redox cycle provides new insights on the nature of the redox processes occurring within a SOC fuel electrode. However, only the initial and final steps of the reactions can be analyzed. To gain information about the intermediate steps of the reduction and oxidation, in-situ holographic tomography is applied. Preliminary results show rapid kinetics for the two reactions. During oxidation, void formation in metallic particles is observed. During reduction, the nickel oxide particles first evolve to a nano-porous system of nickel crystallites and then coarsen towards dense nickel particles.

**General information**

State: Published
Organisations: Department of Energy Conversion and Storage, Imaging and Structural Analysis
Authors: De Angelis, S. (Intern), Bowen, J. R. (Intern), Jørgensen, P. S. (Intern), Lauridsen, E. M. (Intern)
Number of pages: 128
Publication date: 2017

**Publication information**

Publisher: Department of Energy Conversion and Storage, Technical University of Denmark
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions: finalDef2.pdf

**Relations**

Projects:
Tracking Solid Oxide Cell Microstructure Evolution by High Resolution 3D Nano-Tomography
Source: PublicationPreSubmission
Source-ID: 139843599
Publication: Research › Ph.D. thesis – Annual report year: 2017

**Transient deformational properties of high temperature alloys used in solid oxide fuel cell stacks**

Stresses and probability of failure during operation of solid oxide fuel cells (SOFCs) are affected by the deformational properties of the different components of the SOFC stack. Though the overall stress relaxes with time during steady state operation, large stresses would normally appear through transients in operation including temporary shut downs. These stresses are highly affected by the transient creep behavior of metallic components in the SOFC stack. This study investigates whether a variation of the so-called Chaboche's unified power law together with isotropic hardening can represent the transient behavior of Crofer 22 APU, a typical iron-chromium alloy used in SOFC stacks. The material parameters for the model are determined by measurements involving relaxation and constant strain rate experiments. The constitutive law is incorporated into commercial finite element software using a user-defined material model. This is used to validate the developed constitutive law to experiments with constant strain rate, cyclic and creep experiments. The predictions from the developed model are found to agree well with experimental data. It is therefore concluded that Chaboche's unified power law can be applied to describe the high temperature inelastic deformational behaviors of Crofer 22 APU used for metallic interconnects in SOFC stacks.
Transportable Device for Transference of Atmosphere Sensitive Materials from Glove Box to High Resolution Scanning Electron Microscope

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Imaging and Structural Analysis
Authors: Bentzen, J. J. (Intern), Wichmann, M. (Intern), Blanchard, D. (Intern)
Number of pages: 1
Publication date: 2017
Event: Poster session presented at The 68th Annual Conference of the Nordic Microscopy Society (SCANDEM 2017), Reykjavik, Iceland.
Main Research Area: Technical/natural sciences

Electronic versions:
Scandem_2017_poster_jabe.pdf
Source: PublicationPreSubmission
Source-ID: 137101329
Publication: Research › Poster – Annual report year: 2017

Transportable Device for Transference of Atmosphere Sensitive Materials from Glove Box to High Resolution Scanning Electron Microscope

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Imaging and Structural Analysis
Authors: Bentzen, J. J. (Intern), Wichmann, M. (Intern), Blanchard, D. (Intern)
Number of pages: 1
Publication date: 2017
Event: Abstract from The 68th Annual Conference of the Nordic Microscopy Society (SCANDEM 2017), Reykjavik, Iceland.
Main Research Area: Technical/natural sciences
Transfer device, Air sensitive materials, Glove box, HRSEM, High energy battery

Electronic versions:
Scandem2017_abstract_jabe_final.pdf
Source: PublicationPreSubmission
Source-ID: 137101307
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2017

Transport and excitations in a negative-U quantum dot at the LaAlO3/SrTiO3 interface

In a solid-state host, attractive electron–electron interactions can lead to the formation of local electron pairs which play an important role in the understanding of prominent phenomena such as high $T_c$ superconductivity and the pseudogap phase. Recently, evidence of a paired ground state without superconductivity was demonstrated at the level of single electrons in quantum dots at the interface of LaAlO3 and SrTiO3. Here, we present a detailed study of the excitation spectrum and transport processes of a gate-defined LaAlO3/SrTiO3 quantum dot exhibiting pairing at low temperatures. For weak tunneling, the spectrum agrees with calculations based on the Anderson model with a negative effective charging energy $U$, and exhibits an energy gap corresponding to the Zeeman energy of the magnetic pair-breaking field. In contrast, for strong coupling, low-bias conductance is enhanced with a characteristic dependence on temperature, magnetic field and chemical potential consistent with the charge Kondo effect.

General information
Tuning the ground state of polar LaAlO$_3$/SrTiO$_3$ interface by an electron sink

Most of the intriguing properties of two-dimensional electron gases (2DEGs) at the LaAlO$_3$/SrTiO$_3$ (LAO/STO) interface are sensitive to the electrons located in 3d-orbit of Ti. However, tuning the electronic structure of the system remains challenging due to the intrinsic high carrier density. Herein, instead of using LaMnO$_3$ (LMO) as buffer layers [1], we show that Mn doping in LaAlO$_3$ (LAMO) creates an electron sink that alters the ground state of 2DEG by suppressing the carrier density at the interface, without changing the polarity of the system. By precise control of the Mn-doping level, we found that 2DEGs in our system experience a change from two-band to one-band transport with decreasing carrier density, which is accompanied by a Lifshitz transition at a critical carrier density of 2.76×10$^{13}$ cm$^{-2}$ at 2K. Significantly, the peak value (255.7mK) of superconducting transition temperature is observed at Lifshitz point. In addition, our experiments realize the coexistence of ferromagnetism (FM) and superconductivity (SC) by Mn doping.
Tuning the two-dimensional electron liquid at oxide interfaces by buffer-layer-engineered redox reactions

Polar discontinuities and redox reactions provide alternative paths to create two-dimensional electron liquids (2DELs) at oxide interfaces. Herein, we report high mobility 2DELs at interfaces involving SrTiO$_3$ (STO) achieved using polar La$_{7/8}$Sr$_{1/8}$MnO$_3$ (LSMO) buffer layers to manipulate both polarities and redox reactions from disordered overlayers grown at room temperature. Using resonant x-ray reflectometry experiments, we quantify redox reactions from oxide overlayers on STO as well as polarity induced electronic reconstruction at epitaxial LSMO/STO interfaces. The analysis reveals how these effects can be combined in a STO/LSMO/disordered film trilayer system to yield high mobility modulation doped 2DELs, where the buffer layer undergoes a partial transformation from perovskite to brownmillerite structure. This uncovered interplay between polar discontinuities and redox reactions via buffer layers provides a new approach for the design of functional oxide interfaces.
Two-Dimensional Electron Gases at Modulation-doped Oxide Interfaces

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Technical University of Denmark
Number of pages: 1
Publication date: 2017
Event: Abstract from 3rd Functional Oxide Thin Films for Advanced Energy and Information Technology Conference, Rome, Italy.
Main Research Area: Technical/natural sciences
Electronic versions:
abstract_Yunzhong_Modulation_doped_2DEG.pdf
Source: PublicationPreSubmission
Source-ID: 140346906
Publication: Research › Conference abstract for conference – Annual report year: 2017

Two-Dimensional Electron Gases at Modulation-doped Oxide Interfaces

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Technical University of Denmark
Number of pages: 1
Pages: 32
Ultrasensitive binder-free glucose sensors based on the pyrolysis of in situ grown Cu MOF

A non-enzymatic glucose sensor based on carbon/Cu composite materials was developed by the in-situ growth and subsequent pyrolysis of metal-organic frameworks (MOFs) on Cu foam. After pyrolysis, SEM, HRTEM and STEM-EELS were employed to clarify the hierarchical Cu@porous carbon electrode. It is found that the Cu nanoparticles are uniformly embedded in the carbon matrix, attached on the carbon layer closely. The electrocatalytic activity of the Cu@porous carbon matrix electrode for glucose sensing was explored by cyclic voltammetry (CV) and chronamperometry. The resulting Cu@porous carbon matrix electrode displays ultrahigh sensitivity (10.1 mA cm⁻² mM⁻¹), low detection limit (<1 μM), short response time (less than 2 s) and good stability, indicating that the developed electrode is a promising candidate material for glucose sensors.
Ultra-thin Cu2ZnSnS4 solar cell by pulsed laser deposition

We report on the fabrication of a 5.2% efficiency Cu2ZnSnS4 (CZTS) solar cell made by pulsed laser deposition (PLD) featuring an ultra-thin absorber layer (less than 450 nm). Solutions to the issues of reproducibility and micro-particulate ejection often encountered with PLD are proposed. At the optimal laser fluence, amorphous CZTS precursors with optimal stoichiometry for solar cells are deposited from a single target. Such precursors do not result in detectable segregation of secondary phases after the subsequent annealing step. In the analysis of the solar cell device, we focus on the effects of the finite thickness of the absorber layer. Depletion region width, carrier diffusion length, and optical losses due to incomplete light absorption and back contact reflection are quantified. We conclude that material- and junction quality is comparable to that of thicker state-of-the-art CZTS devices, even though the efficiency is lower due to optical losses.

General information

State: Published
Organisations: Department of Photonics Engineering, Optical Microsensors and Micromaterials, Department of Micro- and Nanotechnology, Department of Physics, Experimental Surface and Nanomaterials Physics, Silicon Microtechnology, Department of Energy Conversion and Storage, Electrofunctional materials, The VILLUM Center for the Science for Sustainable Fuels and Chemicals, University of New South Wales, Technical University of Denmark
Authors: Cazzaniga, A. C. (Intern), Crovetto, A. (Intern), Yan, C. (Ekstern), Sun, K. (Ekstern), Hao, X. (Ekstern), Estelrich, J. R. (Ekstern), Canulescu, S. (Intern), Stamate, E. (Intern), Pryds, N. (Intern), Hansen, O. (Intern), Schou, J. (Intern)
Pages: 91–99
Publication date: 2017
Main Research Area: Technical/natural sciences

DOI: 10.1016/j.snb.2017.07.024
Understanding the Capacitance of PEDOT:PSS

Poly(3,4-ethylenedioxythiophene):polystyrene sulfonate (PEDOT:PSS) is the most studied and explored mixed ion-electron conducting polymer system. PEDOT:PSS is commonly included as an electroactive conductor in various organic devices, e.g., supercapacitors, displays, transistors, and energy-converters. In spite of its long-term use as a material for storage and transport of charges, the fundamentals of its bulk capacitance remain poorly understood. Generally, charge storage in supercapacitors is due to formation of electrical double layers or redox reactions, and it is widely accepted that PEDOT-PSS belongs to the latter category. Herein, experimental evidence and theoretical modeling results are reported that significantly depart from this commonly accepted picture. By applying a two-phase, 2D modeling approach it is demonstrated that the major contribution to the capacitance of the two-phase PEDOT-PSS originates from electrical double layers formed along the interfaces between nanoscaled PEDOT-rich and PSS-rich interconnected grains that comprises two phases of the bulk of PEDOT-PSS. This new insight paves a way for designing materials and devices, based on mixed ion-electron conductors, with improved performance.
Unique Crystal Orientation of Poly(ethylene oxide) Thin Films by Crystallization Using a Thermal Gradient

Poly(ethylene oxide), (PEO), thin films of different thicknesses (220, 450, and 1500 nm) and molecular masses (4000, 8000, and 20000 g/mol) have been fabricated by spin-coating of methanol solutions onto glass substrates. All these samples have been recrystallized from the melt using a directional thermal gradient technique. Millimeter-size domains with crystallites uniformly, oriented in the direction of the thermal gradient are observed. Furthermore, the crystallites size and orientation distribution are enhanced (e.g., increases and decreases, respectively) when film thickness is decreased, ultimately leading to a single-crystal-like behavior for 220 nm thick PEO films of mass 8000 g/mol. Interestingly, this fine microstructure is partially retained after melting and subsequent-cooling back to ambient temperature for the highest
molecular weight polymer allowing, in this particular case, to significantly decrease the distribution of crystal orientation obtained after crystallization using the thermal gradient technique.
Universality of electron mobility in LaAlO$_3$/SrTiO$_3$ and bulk SrTiO$_3$

Metallic LaAlO$_3$/SrTiO$_3$ (LAO/STO) interfaces attract enormous attention, but the relationship between the electron mobility and the sheet electron density, $n_s$, is poorly understood. Here, we derive a simple expression for the three-dimensional electron density near the interface, $n_{3D}$, as a function of $n_s$ and find that the mobility for LAO/STO-based interfaces depends on $n_{3D}$ in the same way as it does for bulk doped STO. It is known that undoped bulk STO is strongly compensated with $N$ similar or equal to $5 \times 10^{18}$ cm$^{-3}$ background donors and acceptors. In intentionally doped bulk STO with a concentration of electrons $n_{3D} < N$, background impurities determine the electron scattering. Thus, when $n_{3D} < N$, it is natural to see in LAO/STO the same mobility as in the bulk. On the other hand, in the bulk samples with $n_{3D} > N$, the mobility collapses because scattering happens on $n_{3D}$ intentionally introduced donors. For LAO/STO, the polar catastrophe which provides electrons is not supposed to provide an equal number of random donors and thus the mobility should be larger. The fact that the mobility is still the same implies that for the LAO/STO, the polar catastrophe model should be revisited.
Unlocking the Electrocatalytic Activity of Chemically Inert Amorphous Carbon-Nitrogen for Oxygen Reduction: Discerning and Refactoring Chaotic Bonds

Mild annealing enables inactive nitrogen (N)-doped amorphous carbon (a-C) films abundant with chaotic bonds prepared by magnetron sputtering to become effective for the oxygen reduction reaction (ORR) by virtue of generating pyridinic N. The rhythmic variation of ORR activity elaborates well on the subtle evolution of the amorphous C−N bonds conferred by spectroscopic analysis.

Using Dark Field X-Ray Microscopy To Study In-Operando Yttria Stabilized Zirconia Electrolyte Supported Solid Oxide Cell

Dark Field X-Ray Microscopy is a promising technique to study the structure of materials in nanometer length scale. In combination with x-ray diffraction technique, the microstructure evolution of Yttria Stabilized Zirconia electrolyte based solid oxide cell was studied running at extreme operating conditions.
Using ISOS consensus test protocols for development of quantitative life test models in ageing of organic solar cells

As Organic Photovoltaic (OPV) development matures, the demand grow for rapid characterisation of degradation and application of Quantitative Accelerated Life Tests (QALT) models to predict and improve reliability. To date, most accelerated testing on OPVs has been conducted using ISOS consensus standards. This paper identifies some of the problems in using and interpreting the results for predicting ageing based upon ISOS consensus standard test data. Design of Experiments (DOE) in conjunction with data from ISOS consensus standards are used as the basis for developing life test models for OPV modules. This is used to study their temperature-humidity and light-induced degradation, which enables failure rates during accelerated testing to be assessed against the typical outdoor operational conditions. The life test models are used to assess the relative severity of the ISOS standards and the impact of geographic and seasonal climatic changes on OPV degradation.
Voltage and Thermally Driven Roll-to-Roll Organic Printed Transistor Made in Ambient Air Conditions

Resume: Organic thin film transistors offer great potential for use in flexible electronics. Much of this potential lies in the solution processability of the organic polymers enabling both roll coating and printing on flexible substrates and thus greatly reducing the material and fabrication costs. We present flexible organic power transistors prepared by fast (20 m min⁻¹) roll-to-roll flexographic printing of the drain and source electrode structures, with an interspace below 50 um, directly on polyester foil[1]. The devices have top gate architecture and were completed by slotdie coating of the organic semiconductor poly3hexylthiophene and the dielectric material polyvinylphenol before the gate was applied by screen printing. All the processing was realized in ambient air on a PET flexible substrate. We explore the footprint and the practically accessible geometry of such devices with a special view toward being able to drive large currents while handling the thermal aspects in operation together with other organic printed electronics technologies such as large area organic photovoltaics (OPV) and large area electrochromic displays (EC). We find especially that an elevated operational temperature is beneficial with respect to both transconductance and on/off ratio. We achieve high currents of up to 45 mA at a temperature of 80 °C. Finally, we observe a significant temperature dependence of the performance, which can be explored further in sensing applications.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Organic Energy Materials
Authors: Pastorelli, F. (Intern)
Number of pages: 1
Publication date: 2017
Main Research Area: Technical/natural sciences
Links:

Bibliographical note
Waste to energy plant operation under the influence of market and legislation conditioned changes

In this paper, gate-fee changes of the waste-to-energy plants are investigated in the conditions set by European Union legislation and by the introduction of the new heat market. Waste management and sustainable energy supply are core issues of sustainable development of regions, especially urban areas. These two energy flows logically come together in the combined heat and power facility by waste incineration. However, the implementation of new legislation influences quantity and quality of municipal waste and operation of waste-to-energy systems. Once the legislation requirements are met, waste-to-energy plants need to be adapted to market operation. This influence is tracked by the gate-fee volatility. The operation of the waste-to-energy plant on electricity markets is simulated by using EnergyPLAN and heat market is simulated in Matlab, based on hourly marginal costs. The results have shown that the fuel switch reduced gate-fee and made the facility economically viable again. In the second case, the operation of the waste-to-energy plant on day-ahead electricity and heat market is analysed. It is shown that introducing heat market increased needed gate-fee on the yearly level over the expected levels. Therefore, it can be concluded that the proposed approach can make projects of otherwise questionable feasibility more attractive.
When two become one: an insight into 2D conductive oxide interfaces

Recent progress has led to conductance confinement at the interface of complex oxide heterostructures, thereby providing new opportunities to explore nano-electronic as well as nano-ionic devices. In this paper we describe how interfacial contiguity between materials can trigger redox reactions inducing metallic conductivity along the interface of SrTiO$_3$-based heterostructures and create new types of 2 Dimension Electron Gases (2DEG) at the hetero-interface with electron mobility enhancements of more than one order of magnitude higher than those of hitherto investigated perovskite-type interfaces. Furthermore, our recent results, examining strain effects at interfaces, demonstrate the potential of achieving hetero-epitaxial thin films with superior ionic or electronic properties. We also present a novel concept that uncovers a wide variety of possible technological opportunities for materials design utilizing ionic conducting multi-layered heterostructures. These findings hold the potential to pave the way for novel and/or superior all-oxide electronic and ionic devices.
X-Ray and Raman studies on all-solid-state Li-S batteries built around LiBH4 solid electrolyte
X-Ray microtomography studies on all-solid-state Li-S batteries built around LiBH4 solid electrolyte

General information
State: Published
Organisations: Department of Energy Conversion and Storage
Authors: Lefevr, J. (Intern), Blanchard, D. (Intern)
Number of pages: 1
Publication date: 2017

Host publication information
Title of host publication: Proceedings of the Danscatt Annual meeting 2017
Main Research Area: Technical/natural sciences
Conference: DANS CATT Annual meeting 2017, Odense, Denmark, 01/06/2017 - 01/06/2017
Source-ID: 132365165
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2017

Zirconia nano-colloids transfer from continuous hydrothermal synthesis to inkjet printing
Water dispersions of nanometric yttria stabilized zirconia (YSZ) particles synthesized by Continuous Hydrothermal Synthesis are transferred into nano-inks for thin film deposition. YSZ nanoparticles are synthesized in supercritical conditions resulting in highly dispersed crystals of 10 nm in size. The rheology of the colloid is tailored to achieve inkjet printability (Z) by using additives for regulating viscosity and surface tension. Inks with a wide range of properties are produced. A remarkable effect of nanoparticles on the ink printability is registered even at solid load < 1%vol. In particular, nanoparticles hinder the droplet formation at low values of the printability while suitable jetting is observed at high Z values, i.e. Z ≈ 20. For the optimized inks, we achieve high quality printing with lateral and thickness resolutions of 70 μm and ca. 250 nm respectively, as well as self-leveling effect with a reduction of the substrate roughness. Densification is achieved at sintering temperatures below 1200 °C.

General information
State: Accepted/In press
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Mixed Conductors, Promethean Particles Ltd.
Authors: Rosa, M. (Intern), Gooden, P. N. (Ekstern), Butterworth, S. (Ekstern), Zielke, P. (Intern), Kiebach, W. (Intern), Xu, Y. (Intern), Gadea, C. (Intern), Esposito, V. (Intern)
Number of pages: 25
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of the European Ceramic Society
ISSN (Print): 0955-2219
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
**Partially fluorinated electrospun proton exchange membranes**
The present invention relates to a novel porous membrane layer, to a novel method for producing a membrane, and the membranes produced by the novel method. The present invention further relates to a fuel cell comprising the porous layer, as well as any use of the porous layer in a fuel cell or in a filter. The porous membrane layer comprises a plurality of randomly oriented fibers manufactured by electrospinning, wherein the fibers comprise a graft copolymer, wherein the graft copolymer comprises a backbone and at least one side chain, wherein the backbone comprises a partially fluorinated copolymer, and wherein at least one side chain of the graft copolymer comprises a polymerization product of a polymerizable proton donor group or a precursor thereof.

**General information**
State: Published
Organisations: Department of Chemical and Biochemical Engineering, The Danish Polymer Centre, Department of Energy Conversion and Storage
Authors: Javakhishvili, I. (Intern), Hvilsted, S. (Intern), Jankova Atanasova, K. (Intern)
Publication date: 24 Nov 2016

**Publication information**
IPC: H01M 8/ 10 A I
Patent number: WO2016185009
Date: 24/11/2016
Priority date: 20/05/2015
Original language: English
Main Research Area: Technical/natural sciences
Source: espacenet
Source-ID: WO2016185009
Publication: Research › Patent – Annual report year: 2016

**Gas sensor with multiple internal reference electrodes and sensing electrodes**
The invention relates to a potentiometric gas sensor, or potentiometric gas detection element, with multiple internal reference electrodes and multiple sensing electrodes for determining the concentrations of gas components in a gaseous mixture. The sensor for gas detection comprises: a solid electrolyte, at least two sensing electrodes (SEs) in solid contact with the electrolyte, and at least two internal reference electrodes (IREs) in solid contact with the electrolyte, wherein each IRE comprises a composite material, comprising a binary mixture of a metal and a metal oxide dispersed to form a three-dimensional network extending throughout the IRE, and wherein each SE is electrically connected with at least one IRE.

**General information**
State: Published
Organisations: Department of Energy Conversion and Storage, Fundamental Electrochemistry
Authors: Hu, Q. (Intern), Mogensen, M. B. (Intern)
Publication date: 20 Oct 2016

**Publication information**
IPC: G01N 33/ 00 A I
Patent number: WO2016166126
Date: 20/10/2016
Priority date: 13/04/2015
Original language: English
Main Research Area: Technical/natural sciences
Source: espacenet
Source-ID: WO2016166126
Publication: Research › Patent – Annual report year: 2016

**Dual-role plasticizer and dispersant for ceramic layers**
Thus, one aspect of the invention relates to a green ceramic layer comprising a ceramic material, a binder, and a dual-role dispersant and plasticizer, wherein said dual-role dispersant and plasticizer is an organic di- or tri-ester selected from compounds of formula (I), (II), (III) and (IV). Another aspect of the present invention relates to a slurry for use in the manufacturing of a green ceramic layer comprising a ceramic material, a solvent, a binder, and a dual-role dispersant and
plasticizer, wherein said dual role dispersant and plasticizer is an organic di- or tri-ester. Further aspects include uses of and methods of manufacturing said green ceramic layers.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Risø National Laboratory for Sustainable Energy
Authors: Foghmoes, S. P. V. (Intern), Della Negra, M. (Intern), Klemensø, T. (Intern), Brodersen, K. (Intern)
Publication date: 6 May 2016

Publication information
IPC: C08K 5/11 A I
Patent number: WO2016066173
Date: 06/05/2016
Priority date: 30/10/2014
Priority number: EP20140191072
Original language: English
Electronic versions:
WO2016066173A1.pdf
Main Research Area: Technical/natural sciences
Source: espacenet
Source-ID: WO2016066173
Publication: Research › Patent – Annual report year: 2016

Thermoelectric material comprising scandium doped zinc cadmium oxide
There is presented a composition of scandium doped Zinc Cadmium Oxide with the general formula ZnzCdxScyO which the inventors have prepared, and for which material the inventors have made the insight that it is particularly advantageous as an n-type oxide material, such as particularly advantageous for high temperature thermoelectric application with good TE properties and superior stability in air. In a particular embodiment, there is presented a material with the general formula Zn1-x-yCdxScyO, where 0.05

General information
State: Published
Organisations: Electrofunctional materials, Department of Energy Conversion and Storage, Mixed Conductors, Risø National Laboratory for Sustainable Energy
Authors: Han, L. (Intern), Pryds, N. (Intern), Van Nong, N. (Intern), Linderoth, S. (Intern)
Publication date: 7 Apr 2016

Publication information
IPC: H01L 35/22 A I
Patent number: WO2016050810
Date: 07/04/2016
Priority date: 29/09/2014
Priority number: EP20140186932
Original language: English
Electronic versions:
WO2016050810A1.pdf
Main Research Area: Technical/natural sciences
Source: espacenet
Source-ID: WO2016050810
Publication: Research › Patent – Annual report year: 2016

Polymer solution, fiber mat, and nanofiber membrane-electrode-assembly therewith, and method of fabricating same
In one aspect of the present invention, a fiber mat is provided. The fiber mat includes at least one type of fibers, which includes one or more polymers. The fiber mat may be a single fiber mat which includes one type of fibers, or may be a dual or multi fiber mat which includes multiple types of fibers. The fibers may further include particles of a catalyst. The fiber mat may be used to form an electrode or a membrane. In a further aspect, a fuel cell membrane-electrode-assembly has an anode electrode, a cathode electrode, and a membrane disposed between the anode electrode and the cathode electrode. Each of the anode electrode, the cathode electrode and the membrane may be formed with a fiber mat.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science


2D vs. 1D Structures at Stepped Si Surfaces and In Organic Molecules

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, University of Wisconsin-Madison, Lawrence Berkeley National Laboratory, Naval Research Laboratory, University of Rostock, Universidad del Pais Vasco
Authors: Himpsel, F. (Ekstern), García Lastra, J. M. (Intern), Rubio, Á. (Ekstern), Boukahil, I. (Ekstern), Qiao, R. (Ekstern), Erwin, S. (Ekstern), Barke, I. (Ekstern)
Number of pages: 1
Publication date: 2016
Event: Abstract from Pacific Rim Symposium on Surfaces, Coatings and Interfaces, Kohala Coast, HI, United States.
Main Research Area: Technical/natural sciences
Electronic versions:
2D_vs_1D.pdf
Source: PublicationPreSubmission
Source-ID: 128083371
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2016

3D Mapping Of Density And Crack Propagation Through Sintering Of Catalysis Tablets By X-Ray Tomography

For hydrogen production, by steam reforming, porous ceramics are broadly used as catalyst support, due to their stability and ease in shaping. Catalyst supports in the form of tablets are conventionally produced by powder pressing and subsequent sintering. However, if the process is not done properly, cracks may arise and propagate during the sintering of the tablets. This can lead to weak sintered tablets that get rejected in the quality control. For this work, crack-containing samples of rejected tabletized support were provided. The formation, growth and closure of internal cracks during sintering of the rejected tabletized support material are studied by 3D X-ray tomography. This is a powerful technique, which due to its nondestructive nature is suitable to study the development of internal cracks in the tablets during sintering. Cracks could be identified in the green tablet (before sintering), which may indicate an uneven compaction of the powder, leading to an uneven spring-back after compaction. During sintering, some of the initial cracks were observed to close, while others were observed to open. Furthermore new cracks were also observed to arise during sintering. The different cracks locations and developments were analyzed in relationship to the surrounding microstructural features in an attempt to understand the underlying mechanisms.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Haldor Topsoe AS
Authors: Jacobsen, H. S. (Intern), Puig-Molina, A. (Ekstern), Dalskov, N. (Ekstern), Frandsen, H. L. (Intern)
Number of pages: 8
Publication date: 2016

Host publication information
Title of host publication: Proceedings of the 40th International Conference and Expo on Advanced Ceramics & Composites (ICACC 2016)
Main Research Area: Technical/natural sciences
Conference: 40th International Conference and Exposition on Advanced Ceramics and Composites, Daytona Beach, FL, United States, 24/01/2016 - 24/01/2016
A Cascading Model Of An Active Magnetic Regenerator System

In recent years, significant amounts of studies have been done on modeling and analysis of active magnetic regenerators (AMRs). Depending on the AMR geometry and the magnetocaloric material being modeled, the AMR may not be able to provide the required performance demanded by practical applications. Some AMR models in the literature predict high performance but with relatively low temperature spans at either end of the AMR. Therefore, they may not be sufficient for practical applications, such as providing the heat exchanger temperature spans required for residential and commercial space air conditioning. To remedy this, one solution is cascading of multiple single layer AMRs. In this work, a cascading AMR model is presented and studied. In a cascade configuration, N number of single layer AMRs are connected. The results show that higher hot and cold side temperature differences may be achieved compared to the ones obtained with a single AMR rendering the solution more suitable for use in residential and commercial space conditioning.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, University of Southern Denmark
Pages: 248-251
Publication date: 2016

Host publication information
Title of host publication: Proceedings of the 7th International Conference on Magnetic Refrigeration at Room Temperature
Publisher: International Institute of Refrigeration
Main Research Area: Technical/natural sciences
Cascading model, Active magnetic regenerator, Magnetocaloric material, Temperature span, Practical applications
DOIs:
10.18462/iir.thermag.2016.0194

Accelerated ceria–zirconia solubilization by cationic diffusion inversion at low oxygen activity

Fast elemental diffusion at the Gd-doped ceria/Y-stabilized zirconia interface occurs under reducing conditions at low oxygen activity (pO₂ < 10⁻¹⁵ atm) and high temperature (1400 °C). This effect leads to formation of thick ceria–zirconia solid solution reaction layers in the micro-range vs. thin layers of few tens of nanometers under oxidative conditions (i.e. in synthetic air at pO₂ = 0.21 atm). The fast dissolution occurs by an inversion of the dominating limiting mechanism from the expected Zr⁴⁺ diffusion into the CGO lattice at high pO₂ to an unexpected Ce³⁺ diffusion into the YSZ component under reducing conditions. The diffusion coefficient of 8-fold coordinated Ce³⁺ in YSZ at 1400 °C and pO₂ = 10⁻¹³ atm is estimated to be around 10⁻¹¹ cm² s⁻¹. This value is around 3 orders of magnitude higher than Zr⁴⁺ interdiffusion in CGO under oxidative conditions and about 8 orders of magnitude higher than Ce⁴⁺ self-diffusion in CGO in air at the same temperature.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Imaging and Structural Analysis, Universidade Federal do ABC
Number of pages: 8
Pages: 16871-16878
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Materials Chemistry A
Volume: 4
Issue number: 43
ISSN (Print): 2050-7488
Accelerated creep in solid oxide fuel cell anode supports during reduction

To evaluate the reliability of solid oxide fuel cell (SOFC) stacks during operation, the stress field in the stack must be known. During operation the stress field will depend on time as creep processes relax stresses. The creep of reduced Ni-YSZ anode support at operating conditions has been studied previously. In this work a newly discovered creep phenomenon taking place during the reduction is reported. This relaxes stresses at a much higher rate (∼ x10^4) than creep during operation. The phenomenon was studied both in three-point bending and uniaxial tension. Differences between the two measurements could be explained by newly observed stress promoted reduction. Finally, samples exposed to a small tensile stress (∼ 0.004 MPa) were observed to expand during reduction, which is in contradiction to previous literature. These observations suggest that release of internal residual stresses between the NiO and the YSZ phases occurs during reduction. The accelerated creep should practically eliminate any residual stress in the anode support in an SOFC stack, as has previously been indirectly observed. This phenomenon has to be taken into account both in the production of stacks and in the simulation of the stress field in a stack based on anode supported SOFCs. (C) 2016 Elsevier B.V. All rights reserved.
Acid–Base Chemistry and Proton Conductivity

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors, Case Western Reserve University
Authors: Li, Q. (Intern), Aili, D. (Intern), Savinell, R. F. (Ekstern), Jensen, J. O. (Intern)
Pages: 37-57
Publication date: 2016

Host publication information
Title of host publication: High Temperature Polymer Electrolyte Membrane Fuel Cells: Approaches, Status, and Perspectives
Place of publication: Switzerland
Publisher: Springer
Editors: Li, Q., Aili, D., Hjuler, H. A., Jensen, J. O.
ISBN (Print): 978-3-319-17081-7
ISBN (Electronic): 978-3-319-17082-4
Chapter: 3
Main Research Area: Technical/natural sciences
DOIs: 10.1007/978-3-319-17082-4_3

A contribution to the understanding of the combined effect of nitrogen and boron in grey cast iron

General information
State: Published
Organisations: Department of Mechanical Engineering, Manufacturing Engineering, Department of Energy Conversion and Storage, Mixed Conductors, Dansk Udviklings Formidling ApS
Authors: Strande, K. (Ekstern), Tiedje, N. S. (Intern), Chen, M. (Intern)
Pages: 127-128
Publication date: 2016

Host publication information
Title of host publication: 72nd World Foundry Congress (WFC 2016): Proceedings of a meeting held 21-25 May 2016, Nagoya, Japan.
Publisher: World Foundry Organization
ISBN (Print): 9781510833128
Main Research Area: Technical/natural sciences
Conference: 72nd World Foundry Congress (WFC 2016), Nagoya, Japan, 21/05/2016 - 21/05/2016
Source: FindIt
Source-ID: 2393757283

Active cooling of a down hole well tractor
Wireline interventions in high temperature wells represent one of today’s biggest challenges for the oil and gas industry. The high wellbore temperatures, which can reach 200 °C, drastically reduce the life of the electronic components contained in the wireline downhole tools, which can cause the intervention to fail. Active cooling systems represent a possible solution to the electronics overheating, as they could maintain the sensitive electronics at a tolerable temperature, while operating in hotter environments. This work presents the design, construction and testing of an actively cooled downhole electronics section, which is able to cool the critical electronics below 175 °C while operating at 200 °C. After the investigation of several cooling techniques and the thermal characterization of the studied downhole electronics, thermoelectric coolers were chosen to implement a novel concept of heat management for downhole tools. The chosen design combined active and passive cooling techniques aiming at efficient thermal management, preserving the tool compactness, and avoiding the use of moving parts. Topology optimization was used, in combination with a finite element model of the system, to develop the final design of an actively cooled prototype, which was able to continuously maintain the temperature-sensitive electronics below 170 °C, while operating at 200 °C for more than 200 hours. Effective electrical integration of the cooling system in a wireline downhole tool was also studied, and a power-width-modulation circuit was developed to adapt the downhole power source to a suitable voltage for the thermoelectric cooler. The implementation of
the active cooling system was supported by the study of the thermal interaction between the downhole tool and the well environment, which was relevant to define the heat rejection conditions. Given the lack of information from the scientific literature, a downhole sensor that could experimentally quantify the heat transfer rate occurring between the tool and the wellbore was designed and tested. The concept was proved and the sensor calibrated in a laboratory flow loop. Average and maximum mismatches of 3% and 10%, respectively, were found between the measured and predicted heat transfer coefficients, showing good agreement between experimental results and model forecasts.

---

**General information**

State: Published

Organisations: Department of Energy Conversion and Storage, Electrofunctional materials

Authors: Soprani, S. (Intern), Engelbrecht, K. (Intern), Bahl, C. (Intern), Nesgaard, C. (Ekstern)

Number of pages: 253

Publication date: 2016

**Publication information**

Publisher: Department of Energy Conversion and Storage, Technical University of Denmark

Original language: English

Main Research Area: Technical/natural sciences

Electronic versions:

Stefano_Soprani_PhD_Thesis_2016.pdf

**Relations**

Projects:

Active cooling of a down hole well tractor

Publication: Research › Ph.D. thesis – Annual report year: 2016

---

**Active magnetic regenerator refrigeration with rotary multi-bed technology**

Magnetic refrigeration is an emerging cooling technology with potential advantages over conventional vapor compression, the most important being higher efficiency. This thesis presents experimental and theoretical research into the possibilities of realizing this potential with actual active magnetic regenerator (AMR) prototypes. The starting point is the design and experiments with a rotary multi-bed prototype at the Technical University of Denmark. Promising results were obtained with this machine in terms of temperature span and cooling power. However, issues limiting the energy efficiency, mainly relating to heat leaks and flow system friction losses, have given rise to new ideas for taking the technology a step further. On this background, a second generation multi-bed prototype was designed, built and used in experimental investigations. A central feature of the new prototype is a novel system for handling the heat transfer fluid, providing a reciprocating flow inside the AMR beds while ensuring a continuous unidirectional flow in the surrounding flow circuit, communicating with the hot and cold reservoirs. With this system it is possible, via an arrangement of poppet valves and check valves, to control the flow rate versus rotational angle of the magnet system providing a time varying magnetic field in the beds with very minor losses compared to more traditional rotary valve based systems. Numerical AMR modeling capturing the variations in the azimuthal direction inside the beds has been used to investigate the effect of the shape of this flow profile, which confirms the importance of carefully optimizing it for the desired operating conditions. Numerical modeling and heat transfer calculations addressing heat leaks through the walls of the regenerator housing has revealed a necessary trade off between the amount of magnetocaloric material and an insulating air gap in the magnetized volume provided by the Halbach-like cylindrical permanent magnet system, when designing for high efficiency rather than maximum cooling power. The central part of the magnet system is a flux conducting iron core which was laminated for electrical and thermal insulation to minimize heat leaks and eddy current losses. Experimental investigations with different configurations of iron and insulation in the core focusing on the impact on temperature span and COP were conducted. AMR experiments with the new prototype revealed strong impacts on COP and cooling power by minor adjustments of the individual valves controlling the flow in each bed. This effect, inherent to rotary multibed AMRs, is addressed with a numerical modeling approach and confirmed experimentally with the new prototype by carefully evening out the variations by the means of needle valves. An experimental performance analysis of the new prototype was carried out. A breakdown of the losses indicate pressure drop in external components and regenerator losses as the main contributors to entropy generation. While the former may be reduced by simple design improvements, the latter is non-trivial and requires detailed geometrical optimization assisted by numerical modeling and improved manufacturing techniques. Finally, possible applications are discussed and a concept of operating the AMR machine in combination with a thermal storage is introduced and demonstrated experimentally. Furthermore, a novel shunt valve technology, which was developed as a spin-off from the magnetic refrigeration research, is presented.

---

**General information**

State: Published

Organisations: Department of Energy Conversion and Storage, Electrofunctional materials

Authors: Eriksen, D. (Intern), Engelbrecht, K. (Intern), Bahl, C. (Intern), Bjørk, R. (Intern)

Number of pages: 146

Publication date: 2016
A Decade of Improvements for Solid Oxide Electrolysis Cells. Long-Term Degradation Rate from 40%/Kh to 0.4 % Kh
Solid oxide electrolysis cells (SOEC) have the potential for efficient large-scale conversion from electrical energy to chemical energy stored in fuels, such as hydrogen or synthetic hydrocarbon fuels by use of well-known catalysis processes. Key issues for the break-through of this technology are to provide inexpensive, reliable, high performing and long-term stable SOEC for stack and system applications. At DTU Energy (formerly Department of Fuel Cells and Solid State Chemistry, Risø National Laboratory), research within SOEC for more than a decade has led to long-term degradation rates on cell level being improved from 40 %/kh to 0.4 %/kh for tests at -1 A/cm² (figure 1). In this paper, we review the key findings and highlight different performance and durability limiting factors that have been discovered, analyzed and addressed over the years to reach the tremendous increase in long-term stability for SOEC as illustrated by the cell tests in figure 1.

A Density Functional Theory Study of the Ionic and Electronic Transport Mechanisms in LiFeBO₃ Battery Electrodes
Lithium iron borate is an attractive cathode material for Li-ion batteries due to its high specific capacity and low-cost, earth-abundant constituents. However, experiments have observed poor electrochemical performance due to the formation of an intermediate phase, that is, LiₓFeBO₃, which leads to large overvoltages at the beginning of charge. Using a convex-hull analysis, based on Hubbard-Corrected density functional theory (DFT+U), we identify this intermediate phase as Li₀.5FeBO₃. Moreover, we show by means of the nudged elastic band (NEB) method, that the origin of these adverse electrochemical effects can be explained by an intrinsically low Li-ion and electron/hole-polaron mobility in Li₀.5FeBO₃ due to high activation barriers for both the ionic and electronic transport. These studies include the effects of the experimentally reported commensurate modulation. We have also investigated the Li-ion/hole diffusion through the interface between Li₀.5FeBO₃ and LiFeBO₃, which is found not to result in additional kinetic limitations from Li diffusion across the intraparticle interfaces. These findings suggest that the experimentally observed diminished performance associated with the formation of intermediate phases is linked to the intrinsically poor properties of the Li₀.5FeBO₃ phase rather than to the presence of interfaces between different phases.
A design approach for integrating thermoelectric devices using topology optimization

Efficient operation of thermoelectric devices strongly relies on the thermal integration into the energy conversion system in which they operate. Effective thermal integration reduces the temperature differences between the thermoelectric module and its thermal reservoirs, allowing the system to operate more efficiently. This work proposes and experimentally demonstrates a topology optimization approach as a design tool for efficient integration of thermoelectric modules into systems with specific design constraints. The approach allows thermal layout optimization of thermoelectric systems for different operating conditions and objective functions, such as temperature span, efficiency, and power recovery rate. As a specific application, the integration of a thermoelectric cooler into the electronics section of a downhole oil well intervention tool is investigated, with the objective of minimizing the temperature of the cooled electronics. Several challenges are addressed: ensuring effective heat transfer from the load, minimizing the thermal resistances within the integrated system, maximizing the thermal protection of the cooled zone, and enhancing the conduction of the rejected heat to the oil well. The design method incorporates temperature dependent properties of the thermoelectric device and other materials. The 3D topology optimization model developed in this work was used to design a thermoelectric system, complete with insulation and heat sink, that was produced and tested. Good agreement between experimental results and model forecasts was obtained and the system was able to maintain the load at more than 33 K below the oil well temperature. Results of this study support topology optimization as a powerful design tool for thermal design of thermoelectric systems.
A detailed study of the hysteresis in La_{0.67}Ca_{0.33}MnO_{3}

We report a thorough study of the thermal hysteretic behaviour of a single phase sample of the magnetocaloric material La_{0.67}Ca_{0.33}MnO_{3}. Previous reports in the literature have variously found hysteretic and non-hysteretic behaviour. We show the importance of measuring under carefully defined heating and cooling procedures. Careful analysis of the specific heat, measured at five different temperature ramp rates, and the magnetic entropy change indicates that there is no observable hysteresis, even though the behaviour of both quantities is consistent with a first-order phase transition. We discuss the reasons for this and for the differing results previously found.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Authors: Neves Bez, H. (Intern), Nielsen, K. K. (Intern), Smith, A. (Intern), Bahl, C. R. H. (Intern)
Pages: 429-433
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Magnetism and Magnetic Materials
Volume: 416
ISSN (Print): 0304-8853
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
Advanced Materials for High-Temperature PEM Fuel Cells

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors, Danish Power Systems ApS
Authors: Hjuler, H. A. (Ekstern), Kerr, R. (Ekstern), Steenberg, T. (Ekstern), Terkelsen, C. (Ekstern), Jensen, J. O. (Intern), Cleemann, L. N. (Intern), Li, Q. (Intern)
Number of pages: 1
Publication date: 2016
Main Research Area: Technical/natural sciences
Source: PublicationPreSubmission
Source-ID: 127806948
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2016

Advanced materials for polymer electrolyte membrane fuel cells

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors
Authors: Aili, D. (Intern), Jensen, J. O. (Intern), Li, Q. (Intern)
Pages: 363-383
Publication date: 2016
Host publication information
Title of host publication: Electrochemical Energy: Advanced Materials and Technologies
Place of publication: Boca Raton
Publisher: CRC Press
ISBN (Print): 978-1-4822-2727-7
ISBN (Electronic): 978-1-4822-2728-4
Series: Electrochemical Energy Storage and Conversion
Main Research Area: Technical/natural sciences
Publication: Research - peer-review › Book chapter – Annual report year: 2016

A high mobility two-dimensional electron gas at the CaZrO$_3$/SrTiO$_3$ heterointerface

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Authors: Chen, Y. (Intern), Trier, F. (Intern), Christensen, D. V. (Intern), Linderoth, S. (Intern), Pryds, N. (Intern)
Number of pages: 1
Publication date: 2016
Event: Abstract from TO-BE Spring Meeting 2016, Warwick, United Kingdom.
Main Research Area: Technical/natural sciences
Electronic versions:
A_high_mobility.pdf
Source: PublicationPreSubmission
Source-ID: 127745436
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2016

Al-doped ZnO: RF- or DC-sputtering?

General information
State: Published
Organisations: Department of Micro- and Nanotechnology, Silicon Microtechnology, Department of Energy Conversion and Storage, Fundamental Electrochemistry, Department of Photonics Engineering, Optical Microsensors and
All Metal Organic Deposited High-Tc Superconducting Transition Edge Bolometer on Yttria-Stabilized Zirconia Substrate

We report on the results of a YBa$_2$Cu$_3$O$_{7-x}$ (YBCO) superconductive transition edge bolometer (TEB) fabricated on a Ce$_{0.9}$La$_{0.1}$O$_{2-\delta}$ (CLO) buffered single crystalline yttria-stabilized zirconia (YSZ) substrate. Metal organic deposition was used for the fabrication of both the YBCO thin film as well as CLO buffer layer, while standard photolithography was applied for TEB preparation. YBCO thin film properties were analysed using scanning electron microscopy (SEM), X-ray diffraction (XRD), AC susceptibility and resistance versus temperature measurements. Optical response of the TEB in terms of voltage amplitude and phase was analysed and measured through four-probe technique in a liquid nitrogen cooling system. An increase in voltage amplitude response was observed for the fabricated YBCO/CLO/YSZ bolometer compared to previously reported TEBs with similarly deposited YBCO thin film on a SrTiO$_3$ (STO). This increase is assumed to be a result of the lower thermal conductivity and lower specific heat capacity of YSZ compared to STO substrate.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Sharif University of Technology
Authors: Mohajeri, R. (Ekstern), Opata, Y. A. (Intern), Wulff, A. C. (Intern), Grivel, J. (Intern), Fardmanesh, M. (Ekstern)
Number of pages: 6
Pages: 1981-1986
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Superconductivity and Novel Magnetism
Volume: 30
Issue number: 7
ISSN (Print): 1557-1939
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 1.05 SJR 0.32 SNIP 0.572
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 0.91 SJR 0.332 SNIP 0.544
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.318 SNIP 0.512 CiteScore 0.83
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.381 SNIP 0.613 CiteScore 0.86
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.325 SNIP 0.636 CiteScore 0.83
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
All-solid-state lithium-sulfur battery based on a nanoconfined LiBH₄ electrolyte

In this work we characterize all-solid-state lithium-sulfur batteries based on nano-confined LiBH₄ in mesoporous silica as solid electrolytes. The nano-confined LiBH₄ has fast ionic lithium conductivity at room temperature, 0.1 mS cm⁻¹, negligible electronic conductivity and its cationic transport number (t⁺ = 0.96), close to unity, demonstrates a purely cationic conductor. The electrolyte has an excellent stability against lithium metal. The behavior of the batteries is studied by cyclic voltammetry and repeated charge/discharge cycles in galvanostatic conditions. The batteries show very good performance, delivering high capacities versus sulfur mass, typically 1220 mAh g⁻¹ after 40 cycles at moderate temperature (55°C), 0.03 C rates and working voltage of 2 V.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, Utrecht University
Number of pages: 6
Pages: A2029-A2034
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of the Electrochemical Society
Volume: 163
Issue number: 9
ISSN (Print): 0013-4651
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 3.48 SJR 1.267 SNIP 1.009
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.97 SJR 1.222 SNIP 0.963
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.115 SNIP 1.066 CiteScore 3.17
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.213 SNIP 1.25 CiteScore 3.36
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.169 SNIP 1.309 CiteScore 2.92
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.329 SNIP 1.281 CiteScore 2.61
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.331 SNIP 1.335 CiteScore 2.74
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.418 SNIP 1.304
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.442 SNIP 1.27
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.595 SNIP 1.41
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.569 SNIP 1.322
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.608 SNIP 1.535
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.523 SNIP 1.481
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.712 SNIP 1.7
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.971 SNIP 1.677
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 2.036 SNIP 1.618
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 1.663 SNIP 1.729
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 1.632 SNIP 1.7
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 1.6 SNIP 1.846
Original language: English
All-solid-state battery, Battery, Fast ionic conductor, Lithium sulfur battery, Solid-electrolyte
Electronic versions:
All_Solid_State_Lithium_Sulfur_Battery_Based_on_a_Nanoconfined.pdf
Amino-Functional Polybenzimidazole Blends with Enhanced Phosphoric Acid Mediated Proton Conductivity as Fuel Cell Electrolytes

A new amino-functional polybenzimidazole copolymer is synthesized by homogeneous solution condensation polymerization from a novel monomer, N,N'-bis (2,4-diaminophenyl)-1,3-diaminopropane. The copolymer readily dissolves in organic solvents and shows good film forming characteristics. To balance the phosphoric acid uptake and to obtain mechanically robust membranes, the amino-functional polybenzimidazole derivative is blended with high molecular weight poly [2,2’-(m-phenylene)-5,5’-biphenylbenzimidazole] at different ratios. Due to the high acid uptake, the homogenous blend membranes show enhanced proton conductivity at temperatures well above 100 °C as also confirmed by the fuel cell polarization data.
An Ag based brazing system with a tunable thermal expansion for the use as sealant for solid oxide cells

An Ag-Al2TiO5 composite braze was developed and successfully tested as seal for solid oxide cells. The thermomechanical properties of the Ag-Al2TiO5 system and the chemical compatibility between this composite braze and relevant materials used in stacks were characterized and the leak rates as a function of the operation temperature were measured. The thermal expansion coefficient in the Ag-Al2TiO5 system can be tailored by varying the amount of the ceramic filler. The brazing process can be carried out in air, the joining partners showed a good chemical stability and sufficient low leak rates were demonstrated. Furthermore, the long-term stability of the Ag-Al2TiO5 composite braze was studied under relevant SOFC and SOEC conditions. The stability of brazed Crofer/Ag-Al2TiO5/NiO-YSZ assemblies in reducing atmosphere and in pure oxygen was investigated over 500 h at 850 °C. Additionally, a cell component test was performed to investigate the durability of the Ag-Al2TiO5 seal when exposed to dual atmosphere. The seals performed well over 900 h under electrolysis operation conditions (~0.5 A cm⁻², 850 °C), and no cell degradation related to the Ag-Al2TiO5 sealing was found, indicating that the developed braze system is applicable for the use in SOFC/SOEC stacks.

General information

State: Published
Number of pages: 12
Pages: 339-350
Publication date: 2016
Analysis and comparison of different phase shifters for Stirling pulse tube cryocooler

Investigations of phase shifters and power recovery mechanisms are of sustainable interest for developing Stirling pulse tube cryocoolers (SPTC) with higher power density, more compact design and higher efficiency. This paper investigates the phase shifting capacity and the applications of four different phase shifters, including conventional inertance tube, gas-liquid and spring-oscillator phase shifters, as well as a power recovery displacer. Distributed models based on the electro-acoustic analogy are developed to estimate the phase shifting capacity and the acoustic power dissipation of the three phase shifters without power recovery. The results show that both gas-liquid and spring-oscillator phase shifters have the distinctive capacity of phase shifting with a significant reduction in the inertial component length. Furthermore, full distributed models of SPTCs connected with different phase shifters are developed. The cooling performance of SPTCs using all four phase shifters are presented and typical phase relations are analyzed. The comparison reveals that the power recovery displacer with a more complicated configuration provides the highest efficiency. The gas-liquid and spring-oscillator phase shifters show equivalent efficiency compared with the inertance tube phase shifter. Approximately 10–20% of the acoustic power is dissipated by the phase shifters without power recovery, while 15–20% of the acoustic power can be recovered by the power recovery displacer, leading to a maximum coefficient of performance (COP) above 0.14 at 80 K. A merit analysis is also done by presenting the pros and cons of different phase shifters.

General information

State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, University of Wisconsin-Madison
Authors: Lei, T. (Intern), Pfotenhauer, J. M. (Ekstern), Zhou, W. (Ekstern)
Number of pages: 11
Pages: 63-73
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information

Journal: Cryogenics
Volume: 80
ISSN (Print): 0011-2275
Ratings:
  BFI (2018): BFI-level 1
  Web of Science (2018): Indexed yes
  BFI (2017): BFI-level 1
  Scopus rating (2017): SNIP 1.6 SJR 0.526 CiteScore 1.51
  Web of Science (2017): Indexed Yes
  BFI (2016): BFI-level 1
  Scopus rating (2016): SJR 0.568 SNIP 1.277 CiteScore 1.42
  Web of Science (2016): Indexed yes
  BFI (2015): BFI-level 1
  Scopus rating (2015): SJR 0.474 SNIP 1.466 CiteScore 1.15
  BFI (2014): BFI-level 1
  Scopus rating (2014): SJR 0.475 SNIP 1.286 CiteScore 1.15
  BFI (2013): BFI-level 1
  Scopus rating (2013): SJR 0.457 SNIP 1.109 CiteScore 1.04
  ISI indexed (2013): ISI indexed yes
  BFI (2012): BFI-level 1
  Scopus rating (2012): SJR 0.613 SNIP 1.804 CiteScore 1.08
  ISI indexed (2012): ISI indexed yes
  BFI (2011): BFI-level 1
  Scopus rating (2011): SJR 0.398 SNIP 1.024 CiteScore 0.85
Analysis of diverse direct arylation polymerization (DArP) conditions toward the efficient synthesis of polymers converging with stille polymers in organic solar cells

Despite the emergence of direct arylation polymerization (DArP) as an alternative method to traditional cross-coupling routes like Stille polymerization, the exploration of DArP polymers in practical applications like polymer solar cells (PSCs) is limited. DArP polymers tend to have a reputation for being marginally inferior to Stille counterparts due to the increased presence of defects that result from unwanted side reactions in direct arylation, such as unselective C-H bond activation and homocoupling. We report ten DArP protocols across the three major classes of DArP to generate poly[(2,5-bis(2-hexyldecyloxy)phenylene)-alt-(4,7-di(thiophen-2-yl)benzo[c][1,2,5]thiadiazole)] (PPDTBT). Through evaluation of the method and resulting photophysical and electronic properties, we show not all DArP methods are suitable for generating device-quality alternating copolymers. When DArP PPDTBT was synthesized in superheated THF with Cs2CO3, neodecanoic acid, and P(o-anisyl)3, it generated polymers of exceptional quality that performed comparably to Stille counterparts in both roll coated ITO-free and spin-coated ITO devices.
An Analytical Model for the Influence of Contact Resistance on Thermoelectric Efficiency

An analytical model is presented that can account for both electrical and hot and cold thermal contact resistances when calculating the efficiency of a thermoelectric generator. The model is compared to a numerical model of a thermoelectric leg for 16 different thermoelectric materials, as well as to the analytical models of Ebling et al. (J Electron Mater 39:1376, 2010) and Min and Rowe (J Power Sour 38:253, 1992). The model presented here is shown to accurately calculate the efficiency for all systems and all contact resistances considered, with an average difference in efficiency between the numerical model and the analytical model of -0.07 ± 0.35pp. This makes the model more accurate than previously published models. The maximum absolute difference in efficiency between the analytical model and the numerical model
is 1.14pp for all materials and all contact resistances considered.
A nanoview of battery operation
The redox-active materials in lithium-ion batteries have relatively poor electronic and ionic conduction and may experience stress from charge-discharge volume changes, so their formulation into structures with nanosized features is highly desirable. On page 566 of this issue, Lim et al. (1) characterize individual nanoparticles of the positive electrode material LiFePO$_4$ during charging and discharging. This "in operando" technique ensures that all particles experience the same voltage. The current and lithium concentration are then inferred for individual particles via the change in Fe oxidation state measured during the transformation from LiFePO$_4$ to FePO$_4$ and back.
An axisymmetrical non-linear finite element model for induction heating in injection molding tools

To analyze the heating and cooling phase of an induction heated injection molding tool accurately, the temperature dependent magnetic properties, namely the non-linear B-H curves, need to be accounted for in an induction heating simulation. Hence, a finite element model has been developed, including the non-linear temperature dependent magnetic data described by a three-parameter modified Frohlich equation fitted to the magnetic saturation curve, and solved with an iterative procedure. The numerical calculations are compared with experiments conducted with two types of induction coils, built in to the injection molding tool. The model shows very good agreement with the experimental temperature measurements. It is also shown that the non-linearity can be used without the temperature dependency in some cases, and a proposed method is presented of how to estimate an effective linear permeability to use with simulation codes not able to utilize a non-linear solver. (C) 2015 Elsevier B.V. All rights reserved.
An Electrochemical Impedance Spectroscopy Study on the Effects of the Surface- and Solution-Based Mechanisms in Li-O₂ Cells

The maximum discharge capacity in non-aqueous Li-O₂ batteries has been limited to a fraction of its theoretical value, largely due to a conformal deposition of Li₂O₂ on the cathode surface. However, it has recently been established that additives that increase the shielding of either O₂⁻ or Li⁺ will activate the formation of toroidal shaped Li₂O₂, thereby dramatically increasing cell capacity. Here we apply porous electrode theory to electrochemical impedance measured at the Li-O₂ cathode to investigate changes in the surface- and ionic resistance within the pores under conditions where either the surface-mechanism or the solution-mechanism is favored. Our experimental observations show that (i) an additional charge transfer process is observed in the impedance spectrum where the solution-based mechanism is favored; (ii) that the changes in the ionic resistance in the cathode during discharge (related to Li₂O₂ build up) is much greater in cells where the solution-based mechanism is activated and can qualitatively determine the extent of discharge product deposited within the pores of the cathode versus the deposition extent at the electrode/electrolyte interface; and (iii) that the observed "sudden-death" during discharge is a consequence of the increasing charge transfer resistance.
regardless of whether Li$_2$O$_2$ forms predominantly through either the surface- or solution-based mechanism.
An Electrochemical Impedance Study of the Capacity Limitations In Na–O2 Cells

Electrochemical impedance spectroscopy, pressure change measurements, and scanning electron microscopy were used to investigate the nonaqueous Na–O2 cell potential decrease and rise (sudden deaths) on discharge and charge, respectively. To fit the impedance spectra from operating cells, an equivalent circuit model was used that takes into account the porous nature of the positive electrode and is able to distinguish between the electrolyte resistance in the pores and the charge-transfer resistance of the pore walls. The results obtained indicate that sudden death on discharge is caused by, depending on the current density, either accumulation of large NaO2 crystals that eventually block the electrode surface and/or a thin film of NaO2 forming on the cathode surface at the end of discharge, which limits charge-transfer. The commonly observed sudden rise in potential toward the end of charge may be caused by a concentration depletion of NaO2 dissolved in the electrolyte near the cathode surface and/or an accumulation of degradation products on the cathode surface.

An Electrochemical Impedance Spectroscopy Study on the Effects of the Surface and Solution Based Mechanisms in Li-O2 Cells.pdf

DOIs:
10.1149/2.1111609jes

Bibliographical note
© The Author(s) 2016. Published by ECS. This is an open access article distributed under the terms of the Creative Commons Attribution 4.0 License (CC BY, http://creativecommons.org/licenses/by/4.0/), which permits unrestricted reuse of the work in any medium, provided the original work is properly cited.

Source: FindIt
Source-ID: 2306780545
Publication: Research - peer-review › Journal article – Annual report year: 2016

An Electrochemical Impedance Study of the Capacity Limitations In Na–O2 Cells

Electrochemical impedance spectroscopy, pressure change measurements, and scanning electron microscopy were used to investigate the nonaqueous Na–O2 cell potential decrease and rise (sudden deaths) on discharge and charge, respectively. To fit the impedance spectra from operating cells, an equivalent circuit model was used that takes into account the porous nature of the positive electrode and is able to distinguish between the electrolyte resistance in the pores and the charge-transfer resistance of the pore walls. The results obtained indicate that sudden death on discharge is caused by, depending on the current density, either accumulation of large NaO2 crystals that eventually block the electrode surface and/or a thin film of NaO2 forming on the cathode surface at the end of discharge, which limits charge-transfer. The commonly observed sudden rise in potential toward the end of charge may be caused by a concentration depletion of NaO2 dissolved in the electrolyte near the cathode surface and/or an accumulation of degradation products on the cathode surface.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, Applied Electrochemistry, University of California, Stanford University
Authors: Knudsen, K. B. (Intern), Nichols, J. E. (Ekstern), Vegge, T. (Intern), Luntz, A. C. (Ekstern), McCloskey, B. D. (Ekstern), Hjelm, J. (Intern)
Pages: 10799–10805
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: The Journal of Physical Chemistry Part C
Volume: 120
Issue number: 20
ISSN (Print): 1932-7447
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
An Organic Mixed Ion-Electron Conductor for Power Electronics
A mixed ionic–electronic conductor based on nanofibrillated cellulose compositied with poly(3,4-ethylenedioxythiophene):poly(styrene-sulfonate) along with high boiling point solvents is demonstrated in bulky electrochemical devices. The high electronic and ionic conductivities of the resulting nanopaper are exploited in devices which exhibit record values for the charge storage capacitance (1F) in supercapacitors and transconductance (1S) in electrochemical transistors.
An Organic Mixed Ion–Electron Conductor for Power Electronics

A mixed ionic–electronic conductor based on nanofibrillated cellulose composited with poly(3,4-ethylene-dioxythiophene):poly(styrene-sulfonate) along with high boiling point solvents is demonstrated in bulky electrochemical devices. The high electronic and ionic conductivities of the resulting nanopaper are exploited in devices which exhibit record values for the charge storage capacitance (1F) in supercapacitors and transconductance (1S) in electrochemical transistors.
A platinum-free oxygen reduction catalyst by a one-step pyrolysis process

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors
Authors: Jensen, J. O. (Intern), Hu, Y. (Intern), Zhong, L. (Intern), Pan, C. (Intern), Cleemann, L. N. (Intern), Li, Q. (Intern)
Number of pages: 1
Publication date: 2016
Main Research Area: Technical/natural sciences

A regenerative elastocaloric heat pump
A large fraction of global energy use is for refrigeration and air-conditioning, which could be decarbonized if efficient renewable energy technologies could be found. Vapour-compression technology remains the most widely used system to move heat up the temperature scale after more than 100 years; however, caloric-based technologies (those using the magnetocaloric, electrocaloric, barocaloric or elastocaloric effect) have recently shown a significant potential as alternatives to replace this technology due to high efficiency and the use of green solid-state refrigerants. Here, we report a regenerative elastocaloric heat pump that exhibits a temperature span of 15.3 K on the water side with a corresponding specific heating power up to 800 W kg$^{-1}$ and maximum COP (coefficient-of-performance) values of up to 7. The efficiency and specific heating power of this device exceeds those of other devices based on caloric effects. These results open up the possibility of using the elastocaloric effect in various cooling and heat-pumping applications.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, University of Ljubljana
Authors: Engelbrecht, K. (Intern), Eriksen, D. (Intern), Dallolio, S. (Intern), Tušek, J. (Ekstern), Pryds, N. (Intern)
Number of pages: 1
Publication date: 2016
Main Research Area: Technical/natural sciences

Approaches to a platinum free oxygen reduction catalyst for PEM fuel cells

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors
Authors: Jensen, J. O. (Intern), Hu, Y. (Intern), Zhong, L. (Intern), Pan, C. (Intern), Cleemann, L. N. (Intern), Li, Q. (Intern)
Number of pages: 1
Publication date: 2016
Main Research Area: Technical/natural sciences

Bibliographical note
Oral presentation
Source: PublicationPreSubmission
Source-ID: 127806225
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2016
A stability study of polymer solar cells using conjugated polymers with different donor or acceptor side chain patterns

Improvement of the power conversion efficiency and long term stability remains to be of crucial importance for the further development of polymer solar cells (PSCs). Herein, a donor-acceptor copolymer based on 4,8-di(thiophene-2-yl)benzo[1,2-b:4,5-b']dithiophene (DTBDT) and 4,7-di(thiophene-2-yl)benzo[c][1,2,5]thiadiazole (DTBT), specifically selected because of its suitability for roll-coating in the ambient environment, is investigated in terms of operational stability via partial exchange (5 or 10%) of the alkyl side chain on either the donor or the acceptor monomer with a 2-hydroxyethyl or 2-phenylethyl group. It is shown that the exchange of the hexyl chain on the DTBT moiety has a negative impact on the stability of the polymer as well as on the performance of the resulting PSCs. On the other hand, partial exchange of the 2-hexyldecyl side chain of the BDT unit by a 2-hydroxyethyl group results in an improved photochemical stability of the polymer film and a higher efficiency of 5.6% for the spin-coated PSC. The stability of roll-coated devices also slightly increases with the incorporation of 10% of either the 2-hydroxyethyl or 2-phenylethyl side chain.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Organic Energy Materials, Hasselt University, Vrije Universiteit Brussel
Authors: Heckler, I. M. (Intern), Kesters, J. (Ekstern), Defour, M. (Ekstern), Penxten, H. (Ekstern), Van Mele, B. (Ekstern), Maes, W. (Ekstern), Bundgaard, E. (Intern)
Number of pages: 13
Pages: 16677-16689
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Materials Chemistry A
Volume: 4
Issue number: 42
ISSN (Print): 2050-7488
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 9.61 SJR 3.488 SNIP 1.55
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 8.46 SJR 3.075 SNIP 1.479
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 2.62 SNIP 1.643 CiteScore 8.36
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
A systematic approach applied in design of a micro heat exchanger

The number of products benefiting from micro components in the market is increasing, and consequently, the demand for well-matched tools, equipment and systems with micro features is eventually increasing as well. During the design process of micro products, a number of issues appear which are inherent due to the down scaling or physical phenomena dominating in the micro range but negligible in the macro scale. In fact, some aspects in design for micro manufacturing are considerably different compared to the de- sign procedure taken at the macro level. Identifying the differences between design considerations at micro compared to macro scale, and defining potential guidelines based on them, provides an opportunity to modify the conventional design methodologies towards becoming micro specific. In this paper, the need for a micro-oriented approach for designing micro products which has not been investigated hitherto studied.

For this purpose, an additional step named "Rules To Consider" (RTC) is added to the conventional design methodologies. This step is constituted based on the feedbacks gained during analyzing the different iterations of the design. The knowledge obtained during the design process of a micro product can be added to the RTC unit, and this unit becomes enriched progressively in design process of similar micro products and supplemented to the conventional design methodologies to be served as a micro-oriented design methodology. In order to present the application of RTC unit, the design process of a micro heat exchanger is investigated. Manufacturability and functional performance are considered as evaluation criteria, and the lessons learned from each design iteration and evaluation are employed in the subsequent design proposals until an acceptable design is achieved. Thermal performance of the heat exchangers is evaluated using finite element (FE) simulation of the conjugate heat transfer. The design proposals are optimized in terms of geometric dimensions, and a sensitivity analysis is conducted on the mass flow rate and heat generation power in the heat source. Finally, the designs with higher thermal performance and manufacturability are introduced. The result of the thermal analysis reveals the fact that the presence of the fins and modification of their dimensions as well as the constituent material for fabricating the micro heat exchanger do not significantly improve the thermal performance of the micro heat exchangers. This is an interesting outcome which can result in considerable reduction of the manufacturing costs by simplifying the geometrical design of the heat exchanger. The micro-specific design considerations which are extracted from the design process of the micro heat exchanger are added to the RTC unit and can be applied as guidelines in design process of any other micro heat exchanger. In other words, the current study can provide a useful guideline in design for manufacturing of micro products.
A TEM study of morphological and structural degradation phenomena in LiFePO$_4$-CB cathodes: Morphological and structural degradation in LiFePO$_4$-CB cathodes

LiFePO$_4$-based cathodes suffer from various degradation mechanisms, which influences the battery performance. In this paper, morphological and structural degradation phenomena in laboratory cathodes made of LiFePO$_4$ mixed with carbon black (CB) in a 1 mol/L LiPF$_6$ in EC:DMC (1:1 by weight) electrolyte are investigated by transmission electron microscopy at various preparation, assembling, storage, and cycling stages. High-resolution transmission electron microscopy imaging shows that continuous SEI layers are formed on the LiFePO$_4$ particles and that both storage and cycling affect the formation. Additionally, loss of CB crystallinity, CB aggregation, and agglomeration is observed. Charge–discharge curves...
and impedance spectra measured during cycling confirm that these degradation mechanisms reduce the cathode conductivity and capacity.

**General information**

State: Published
Organisations: Department of Energy Conversion and Storage, Imaging and Structural Analysis, Applied Electrochemistry
Authors: Ngo, D. (Intern), Scipioni, R. (Intern), Simonsen, S. B. (Intern), Jørgensen, P. S. (Intern), Jensen, S. H. (Intern)
Number of pages: 11
Pages: 2022-2032
Publication date: 2016
Main Research Area: Technical/natural sciences

**Publication information**

Journal: International Journal of Energy Research
Volume: 40
Issue number: 14
ISSN (Print): 0363-907X
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 0.941 SJR 0.764 CiteScore 2.72
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.44 SJR 0.744 SNIP 0.891
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.889 SNIP 1.06 CiteScore 2.52
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.034 SNIP 1.338 CiteScore 2.56
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.043 SNIP 1.641 CiteScore 2.71
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.076 SNIP 1.412 CiteScore 2.2
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.012 SNIP 1.349 CiteScore 2.24
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.114 SNIP 1.325
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.027 SNIP 1.208
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.589 SNIP 0.778
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.584 SNIP 1.012
Scopus rating (2006): SJR 0.727 SNIP 0.836
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.043 SNIP 0.84
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.872 SNIP 0.939
Scopus rating (2003): SJR 0.582 SNIP 0.616
Scopus rating (2002): SJR 0.457 SNIP 0.594
Scopus rating (2001): SJR 0.75 SNIP 0.724
Scopus rating (2000): SJR 0.686 SNIP 0.629
A thermoelectric power generating heat exchanger: Part I – Experimental realization

An experimental realization of a heat exchanger with commercial thermoelectric generators (TEGs) is presented. The power producing capabilities as a function of flow rate and temperature span are characterized for two different commercial heat transfer fluids and for three different thermal interface materials. The device is shown to produce 2W per TEG or 0.22W cm⁻² at a fluid temperature difference of 175 °C and a flow rate per fluid channel of 5 L min⁻¹. One experimentally realized design produced 200W in total from 100 TEGs. For the design considered here, the power production is shown to depend more critically on the fluid temperature span than on the fluid flow rate. Finally, the temperature span across the TEG is shown to be 55–75% of the temperature span between the hot and cold fluids. © 2016 Elsevier Ltd. All rights reserved.
In Part I of this study, the performance of an experimental integrated thermoelectric generator (TEG)-heat exchanger was presented. In the current study, Part II, the obtained experimental results are compared with those predicted by a finite element (FE) model. In the simulation of the integrated TEG-heat exchanger, the thermal contact resistance between the TEG and the heat exchanger is modeled assuming either an ideal thermal contact or using a combined Cooper–Mikic–Yovanovich (CMY) and parallel plate gap formulation, which takes into account the contact pressure, roughness and hardness of the interface surfaces as well as the air gap thermal resistance at the interface. The combined CMY and parallel plate gap model is then further developed to simulate the thermal contact resistance for the case of an interface material. The numerical results show good agreement with the experimental data with an average deviation of 17% for the case without interface material and 12% in the case of including additional material at the interfaces. The model is then employed to evaluate the power production of the integrated system using different interface materials, including graphite, aluminum (Al), tin (Sn) and lead (Pb) in a form of thin foils. The numerical results show that lead foil at the interface has the best performance, with an improvement in power production of 34% compared to graphite foil. Finally, the model predicts that for a certain flow rate, increasing the parallel TEG channels for the integrated systems with 4, 8, and 12TEGs enhances the net power per TEG with average values of 2.5%, 3% and 5%, respectively. © 2016 Elsevier Ltd. All rights reserved.
Main Research Area: Technical/natural sciences

Publication information
Journal: Energy Conversion and Management
Volume: 119
ISSN (Print): 0196-8904
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 6.85 SJR 2.537 SNIP 2.233
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 6.04 SJR 2.232 SNIP 2.109
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 2.023 SNIP 2.079 CiteScore 5.24
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.789 SNIP 2.791 CiteScore 5.35
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.613 SNIP 2.534 CiteScore 4.49
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.674 SNIP 2.242 CiteScore 3.72
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.24 SNIP 1.82 CiteScore 3.03
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.35 SNIP 1.735
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.302 SNIP 1.798
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.471 SNIP 1.886
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.186 SNIP 1.807
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.294 SNIP 1.797
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.542 SNIP 1.769
Scopus rating (2004): SJR 1.043 SNIP 1.467
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 0.879 SNIP 1.382
Scopus rating (2002): SJR 0.972 SNIP 1.467
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.794 SNIP 0.86
Scopus rating (2000): SJR 0.568 SNIP 0.72
Scopus rating (1999): SJR 0.512 SNIP 0.731
Attempts at doping indium in MgB$_2$

Indium (In) doped MgB$_2$ polycrystalline samples were prepared by solid-liquid phase reaction in Ar. After reaction at 800 °C, less than 1 at.% Mg was replaced by In in the MgB$_2$ phase, without significant influence on its lattice parameters and only a slight decrease of its superconducting transition temperature. For all studied In concentrations in the nominal composition, the formation of InMg was evidenced by X-ray diffraction. The critical current density and accommodation field of the wires are decreased in the samples containing In. The flux pinning mechanism can be described by surface pinning in both the doped and undoped samples.
A Two-Level Undercut-Profile Substrate for Chemical-Solution-Based Filamentary Coated Conductors

A recently developed two-level undercut-profile substrate (2LUPS), containing two levels of plateaus connected by a curved wall with an undercut profile, enables self-forming filaments in a coated conductor during physical line-of-sight deposition of buffer and superconducting layers. In the present study, the 2LUPS concept is applied to a commercial cube-textured Ni-5at.% W tape, and the surface of the 2LUPS coated with two Gd2Zr2O7 buffer layers using chemical solution deposition is examined. Except for narrow regions near the edge of upper plateaus, the plateaus are found to be covered by strongly textured Gd2Zr2O7 buffer layers after dip coating and sintering.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Department of Wind Energy, Materials science and characterization, SUBRA IVS, Sharif University of Technology
Authors: Wulff, A. C. (Intern), Lundeman, J. H. (Ekstern), Hansen, J. B. (Ekstern), Mishin, O. (Intern), Yue, Z. (Intern), Mohajeri, R. (Ekstern), Grivel, J. (Intern)
Number of pages: 4
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: IEEE Transactions on Applied Superconductivity
Volume: 26
Issue number: 3
Article number: 6601604
ISSN (Print): 1051-8223
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 1.45 SJR 0.408 SNIP 0.962
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.42 SJR 0.398 SNIP 1.145
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.403 SNIP 1.06 CiteScore 1.27
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.478 SNIP 1.13 CiteScore 0.83
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.443 SNIP 1.156 CiteScore 1.32
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.555 SNIP 1.274 CiteScore 1.11
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.368 SNIP 1.062 CiteScore 1.16
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.473 SNIP 1.065
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.447 SNIP 1.021
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.884 SNIP 0.981
Scopus rating (2007): SJR 0.629 SNIP 1.093
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 0.734 SNIP 1.05
Scopus rating (2005): SJR 0.652 SNIP 0.992
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.882 SNIP 0.904
Scopus rating (2003): SJR 0.51 SNIP 1.054
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 1.226 SNIP 1.024
Scopus rating (2001): SJR 0.552 SNIP 1.368
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 0.498 SNIP 0.998
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 1.054 SNIP 2.065

Original language: English

Etching, Scanning electron microscopy, Substrates, Superconducting filaments and wires, Texture

Electronic versions: A_Two_Level_Undercut_Profile_Substrate_for_Chemical_Solution_Based_Filamentary_Coated_Conductors_postprint.pdf
DOIs: 10.1109/TASC.2016.2536938

Bibliographical note
(c) 2016 IEEE. Personal use of this material is permitted. Permission from IEEE must be obtained for all other users, including reprinting/republishing this material for advertising or promotional purposes, creating new collective works for resale or redistribution to servers or lists, or reuse of any copyrighted components of this work in other works.

Source: FindIt
Source-ID: 2295552108
Publication: Research - peer-review › Journal article – Annual report year: 2016
A viable electrode material for use in microbial fuel cells for tropical regions

Electrode materials are critical for microbial fuel cells (MFC) since they influence the construction and operational costs. This study introduces a simple and efficient electrode material in the form of palm kernel shell activated carbon (AC) obtained in tropical regions. The novel introduction of this material is also targeted at introducing an inexpensive and durable electrode material, which can be produced in rural communities to improve the viability of MFCs. The maximum voltage and power density obtained (under 1000 Ω load) using an H-shaped MFC with AC as both anode and cathode electrode material was 0.66 V and 1.74 W/m³, respectively. The power generated by AC was as high as 86% of the value obtained with the extensively used carbon paper. Scanning electron microscopy and Denaturing Gradient Gel Electrophoresis (DGGE) analysis of AC anode biofilms confirmed that electrogenic bacteria were present on the electrode surface for substrate oxidation and the formation of nanowires.
Baselines for Lifetime of Organic Solar Cells

The process of accurately gauging lifetime improvements in organic photovoltaics (OPVs) or other similar emerging technologies, such as perovskites solar cells is still a major challenge. The presented work is part of a larger effort of developing a worldwide database of lifetimes that can help establishing reference baselines of stability performance for OPVs and other emerging PV technologies, which can then be utilized for pass-fail testing standards and predicting tools. The study constitutes scanning of literature articles related to stability data of OPVs, reported until mid-2015 and collecting the reported data into a database. A generic lifetime marker is utilized for rating the stability of various reported devices. The collected data is combined with an earlier developed and reported database, which was based on articles reported until mid-2013. The extended database is utilized for establishing the baselines of lifetime for OPVs tested under different conditions. The work also provides the recent progress in stability of unencapsulated OPVs with different architectures, as well as presents the updated diagram of the reported record lifetimes of OPVs. The presented work is another step forward towards the development of pass-fail testing standards and lifetime prediction tools for emerging PV technologies.

General information

State: Published
Organisations: Department of Energy Conversion and Storage, Organic Energy Materials, Functional organic materials, ICFO - Institute of Photonic Sciences, University of Minho, Zurich University of Applied Sciences, CNRS, Institut Català de Nanociència i Nanotecnologia, Technische Universität Ilmenau, Cyprus University of Technology, Imperial College London
Number of pages: 9
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Advanced Energy Materials
Volume: 6
Issue number: 22
ISSN (Print): 1614-6832
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 16.78 SJR 8.23 SNIP 2.347
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 12.96 SJR 6.515 SNIP 2.14
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 6.219 SNIP 2.546 CiteScore 14.2
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 6.668 SNIP 2.942 CiteScore 15.27
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 6.006 SNIP 2.949 CiteScore 13.24
Beneficial Effect of Surface Decorations on the Surface Exchange of Lanthanum Strontium Ferrite and Dual Phase Composites

Perovskites within the (La,Sr)(Fe,Co)O3 class of materials show variations in the oxygen stoichiometry depending on temperature and oxygen activity and can potentially be used as catalysts, electrodes in high-temperature solid oxide fuel cells, gas sensors or for oxygen transport membranes. These perovskites possess a mixed ionic and electronic conductivity (MIEC), which can be highly beneficial for the processes on oxygen electrode surfaces. The oxygen transport through a MIEC is determined by the rate of the oxygen exchange over the gas-solid interface and the diffusivity of oxide ions and electrons (or holes) in the bulk. The oxygen exchange process over the surface in general involves several reaction steps, O2 adsorption, dissociation, charge transfer and incorporation of ionic species. The Co-free end member of the material class; LSF (e.g. (La0.6Sr0.4FeO3-δ) is fairly low cost and chemically stable in both mildly reducing and oxidizing atmosphere. The electronic conductivity is excellent (283 S/cm at 800 °C) but the ionic conductivity especially at low temperature is limited (0.014 S/cm, 800 °C). Due to these properties the material is a candidate for use in composite membranes in combination with a better ionic conducting material like CGO. Such systems are also excellent model systems for fundamental studies of the oxygen exchange process.
Benefits of Integrating Geographically Distributed District Heating Systems

Although liberalization of the electricity day-ahead markets has gained pace throughout the Europe, district heating markets are often dominated by lack of competition between suppliers, which curbs the potential of having cheaper systems in terms of socio-economic costs, and technically better system in terms of CO2 emissions. In order to assess the financial and technical outcome of connecting five adjacent district heating systems, a linear continuous optimization model that minimizes total socio-economic costs was developed. Geographical distribution of different district heating systems was truly represented. The model was adapted to the case of Sønderborg municipality in Denmark and the results show that three out of four interconnections are economic feasible in the present system. In the reference year (2013) total system costs were 4.1 % lower, while total primary energy supply was reduced by 1.76 %. For the year 2029, in which intermittent renewable energy sources are dominating the energy generation, total socio-economic costs were reduced by 5.9 %, CO2 emissions by 7.1 % and primary energy supply by 8.4 % after the adjacent district heating systems were connected. Hence, the integration of district heating systems have beneficial impact on the integration of intermittent renewable energy sources.

General information
State: Published
Organisations: Centre for IT-Intelligent Energy Systems in Cities, Department of Energy Conversion and Storage, Aalborg University, University of Zagreb
Authors: Dominkovic, D. F. (Intern), Bačeković, I. (Ekstern), Sveinbjörnsson, D. Þ. (Intern), Pedersen, A. S. (Intern), Krajačić, G. (Ekstern)
Number of pages: 1
Publication date: 2016

Host publication information
Title of host publication: Proceedings of ECOS 2016 : 29th International Conference on Efficiency, Cost, Optimization, Simulation and Environmental Impact of Energy Systems
Main Research Area: Technical/natural sciences
Conference: 29th International Conference on Efficiency, Cost, Optimization, Simulation and Environmental Impact of Energy Systems, Portorož, Slovenia, 19/06/2016 - 19/06/2016
Local communities, CO2, Renewable energy, Systems, Energy system optimization, GIS, Zero carbon
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2016

Beyond the top of the volcano? - A unified approach to electrocatalytic oxygen reduction and oxygen evolution

We study the oxygen reduction (ORR) and the oxygen evolution reaction (OER) and based on previous obtained mechanistic insight we provide a unified general analysis of the two reactions simultaneously. The analysis shows that control over at least two independent binding energies is required to obtain a reversible perfect catalyst for both ORR and OER. Often only the reactivity of the surface is changed by changing from one material to another and all binding energies scale with the reactivity. We investigate the limitation in efficiency imposed by these linear scaling relations. This analysis gives rise to a double volcano for ORR and OER, with a region in between, forbidden by the scaling relations. The reversible perfect catalyst for both ORR and OER would fall into this “forbidden region”. Previously, we have found that hydrogen acceptor functionality on oxide surfaces can improve the catalytic performance for OER beyond the limitations originating from the scaling relations. We use this concept to search for promising combinations of binding sites and hydrogen donor/acceptor sites available in transition metal doped graphene, which can act as a catalyst for ORR and OER. We find that MnN4-site embedded in graphene by itself or combined with a COOH is a promising combination for a great combined ORR/OER catalyst.

General information
State: Published
Organisations: Department of Physics, Department of Energy Conversion and Storage, Atomic scale modelling and materials, Technical University of Darmstadt, University of Copenhagen
Authors: Busch, M. (Intern), Halck, N. B. (Intern), Kramm, U. I. (Ekstern), Siahrostami, S. (Intern), Krtil, P. (Ekstern), Rossmeisl, J. (Ekstern)
Number of pages: 10
Pages: 126–135
Publication date: 2016
Main Research Area: Technical/natural sciences
Heterogeneous catalysis studies were conducted on two crushed solid oxide fuel cell (SOFC) anodes in fixed-bed reactors. The baseline anode was Ni/ScYSZ (Ni/scandia and yttria stabilized zirconia), the other was Ni/ScYSZ modified with Pd/doped ceria (Ni/ScYSZ/Pd-CGO). Three main types of experiments were performed to study catalytic activity and effect of sulfur poisoning: (i) CH₄ and CO₂ dissociation; (ii) biogas (60% CH₄ and 40% CO₂) temperature-programmed reactions (TPRxn); and (iii) steady-state biogas reforming reactions followed by postmortem catalyst characterization by temperature-programmed oxidation and time-of-flight secondary ion mass spectrometry. Results showed that Ni/ScYSZ/Pd-CGO was more active for catalytic dissociation of CH₄ at 750°C and subsequent reactivity of deposited carbonaceous species. Sulfur deactivated most catalytic reactions except CO₂ dissociation at 750°C. The presence of Pd-CGO helped to mitigate sulfur deactivation effect; e.g. lowering the onset temperature (up to 190°C) for CH₄ conversion during temperature-programmed reactions. Both Ni/ScYSZ and Ni/ScYSZ/Pd-CGO anode catalysts were more active for dry reforming of biogas than they were for steam reforming. Deactivation of reforming activity by sulfur was much more severe under steam reforming conditions than dry reforming; a result of greater sulfur retention on the catalyst surface during steam reforming.
Can We Replace Platinum Metals in PEM Fuel Cells and Electrolyzers?

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors
Authors: Jensen, J. O. (Intern), Hu, Y. (Intern), Zhong, L. (Intern), Pan, C. (Intern), Cleemann, L. N. (Intern), Li, Q. (Intern)
Capturing metal-support interactions in situ during the reduction of a Re promoted Co/γ-Al₂O₃ catalyst

The reduction of a Re promoted Co/γ-Al₂O₃ catalyst was monitored in situ by synchrotron X-ray powder diffraction (XRPD) under H₂ environment. Whole powder pattern analysis revealed a non-linear expansion of the unit cell of γ-Al₂O₃ during the reduction process, suggesting the diffusion of Co cations into the structure of the support. The non-linear cell expansion coincided with the formation of a CoO phase. In addition, space resolved diffraction at the inlet and the outlet of the reactor evidenced a negative effect of the partial pressure of indigenous H₂O(g) on the reduction process.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, European Synchrotron Radiation Facility, Norwegian University of Science and Technology, SINTEF
Authors: Tsakoumis, N. E. (Ekstern), Johnsen, R. E. (Intern), van Beek, W. (Ekstern), Rønning, M. (Ekstern), Rytter, E. (Ekstern), Holmen, A. (Ekstern)
Number of pages: 4
Pages: 3239-3242
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Chemical Communications
Volume: 52
Issue number: 15
ISSN (Print): 1359-7345
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 6.03 SJR 2.555 SNIP 1.127
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 6.06 SJR 2.538 SNIP 1.16
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 2.601 SNIP 1.295 CiteScore 6.7
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.692 SNIP 1.436 CiteScore 6.83
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.752 SNIP 1.372 CiteScore 6.73
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 3.118 SNIP 1.35 CiteScore 6.21
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 2.889 SNIP 1.323 CiteScore 5.96
To solve issues of coking and redox instability related to the presence of nickel in typical fuel electrodes in solid oxide cells, Gd-doped CeO$_2$ (CGO) electrodes were studied using symmetric cells. These electrodes showed high electrocatalytic activity, but low electronic conductivity. When infiltrated with Sr$_{0.99}$Fe$_{0.75}$Mo$_{0.25}$O$_{3-\delta}$ (SFM), the electronic conductivity was enhanced. However, polarization resistance of the cells increased, suggesting that the infiltrated material is less electro-catalytically active and was partly blocking the CGO surface reaction sites. The activity could be regained by infiltrating nano-sized CGO or NiCGO on top of SFM, while still sustaining the high electronic conductivity. Ohmic resistance of the electrodes was thus practically eliminated and performance comparable to, or better than, state-of-the-art fuel electrodes was achieved. The Ni containing cells were damaged by carbon deposition in a CO/CO$_2$ atmosphere, while none of the non-nickel cells catalyzed carbon. Stability towards redox cycles was also proven.
Ceramic tape casting: A review of current methods and trends with emphasis on rheological behaviour and flow analysis

Tape casting has been used to produce thin layers of ceramics that can be used as single layers or can be stacked and laminated into multilayered structures. Today, tape casting is the basic fabrication process that provides multilayered capacitors and multilayered ceramic packages. In tape casting the rheological behaviour of the slurry as well as the material flow during casting are of utmost importance since these phenomena to a large extent determine the final properties and hence the quality of the cast product. During the last decades this has led to an increasing number of works in literature within fluid flow analysis of tape casting. In the present paper a review of the development of the tape casting process with particular focus on the rheological classifications as well as modelling the material flow is hence presented and in this context the current status is examined and future potential discussed.
Challenges in going from 2nd order to 1st order materials in magnetic refrigeration devices
Challenges in Membrane Electrode Assembly Technologies

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors
Authors: Jensen, J. O. (Intern), Hu, Y. (Intern), Zhong, L. (Intern), Cleemann, L. N. (Intern), Li, Q. (Intern)
Number of pages: 1
Publication date: 2016
Main Research Area: Technical/natural sciences

Bibliographical note
Invited plenary talk
Source: PublicationPreSubmission
Source-ID: 127805790
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2016

Characterisation of a Planar Solid Oxide Cell Stack Operated at Elevated Pressure

As the global and local energy production becomes more dependent on intermittent renewable sources like wind and solar, efficient and reversible conversion of electricity to storable fuels becomes increasingly important. Solid oxide cells (SOCs) are interesting in this context since they can be operated either as electrolysers (SOEC) to convert electricity to fuels such as hydrogen or methane, and as fuel cells (SOFC) to convert fuels to electricity. Both productivity and conversion efficiency can be improved if the SOC operation pressure can be increased from ambient pressure to 10-30 bar.

Here we characterize an SOC stack operated at pressures from ambient pressure to 10 bar without fluctuations in the steam supply. The pressure dependency of stack temperature, cell area specific resistance (ASR), current-voltage (IV) curves, stack impedance spectra and pressure drop across the stack and heat exchangers is analyzed and the expected impact of pressurization on the hydrogen production cost is evaluated.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry, Mixed Conductors, Haldor Topsoe AS
Authors: Jensen, S. H. (Intern), Graves, C. R. (Intern), Chen, M. (Intern), Sun, X. (Intern), Hansen, J. B. (Ekstern)
Publication date: 2016
Conference: PRIME 2016/230th ECS Meeting, Honolulu, United States, 02/10/2016 - 02/10/2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Electrochemical Society. Meeting Abstracts (Online)
Volume: MA2016-02
Article number: 3077
ISSN (Print): 2151-2043
Original language: English
Links:
http://ma.ecsd.org.proxy.findit.dtu.dk/content/MA2016-02/40/3077.abstract?sid=92d73baa-3694-4497-ad3b-bfb3b4013b9b
Characterization and modeling of organic (P3HT:PCBM) solar cells as a function of bias and illumination

We investigated the response of roll coated organic solar cells at different bias voltages and illumination levels to implement a detailed impedance model. The technique used for the investigation is based on the combination of standard DC characterization with the impedance spectroscopy at different bias and illumination intensity conditions. We analyzed both fresh and intentionally degraded cells. The impedance spectra show different peaks evolutions, depending on the degradation of the cells. Moreover, the same trend appears by measuring the cell at different illumination levels. To describe the cell impedance behaviors we suggest an electrical model based on distributed elements. By fitting the model to experimental data, we extrapolate the parameters related to electron transport, recombination and accumulation. The main differences between fresh and degraded samples are underlined. (C) 2016 Elsevier B.V. All rights reserved.

General information
State: Published
Number of pages: 9
Pages: 337-345
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Volume: 157
ISSN (Print): 0927-0248
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 4.83 SJR 1.459 SNIP 1.532
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.97 SJR 1.599 SNIP 1.71
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.8 SNIP 1.851 CiteScore 5.16
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.19 SNIP 2.348 CiteScore 5.87
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 2.179 SNIP 2.529 CiteScore 5.58
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.441 SNIP 2.654 CiteScore 5.25
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.182 SNIP 2.577 CiteScore 5.16
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 2.494 SNIP 2.105
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Characterization of a Planar Solid Oxide Cell Stack Operated at Elevated Pressure

As global and local energy production becomes more dependent on intermittent renewable sources like wind and solar, efficient and reversible conversion of electricity to storable fuels becomes increasingly important. Solid oxide cells (SOCs) are interesting in this context since they can be operated either as electrolyzers (SOEC) to convert electricity to fuels such as hydrogen or methane, and as fuel cells (SOFC) to convert fuels to electricity. Both productivity and conversion efficiency can be improved if the SOC operation pressure can be increased from ambient pressure to 10–30 bar. In this paper we characterize an SOC stack operated at pressures from ambient pressure to 10 bar. The pressure dependency of stack temperature, cell area specific resistance (ASR), current-voltage (iV) curves, stack impedance spectra and pressure drop across the stack and heat exchangers is analyzed in this paper. Additionally, the expected impact on the hydrogen production efficiency and cost is discussed.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry, Mixed Conductors, Haldor Topsoe AS
Authors: Jensen, S. H. (Intern), Graves, C. R. (Intern), Chen, M. (Intern), Hansen, J. B. (Ekstern), Sun, X. (Intern)
Number of pages: 9
Pages: F1596-F1604
Publication date: 2016
Conference: PRIME 2016/230th ECS Meeting, Honolulu, United States, 02/10/2016 - 02/10/2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of The Electrochemical Society
Volume: 163
Issue number: 14
ISSN (Print): 0013-4651
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Characterization Of Biaxial Strain Of Poly(L-Lactide) Tubes

Poly(L-lactide) (PLLA) in its L-form has promising mechanical properties. Being a semi-crystalline polymer, it can be subjected to strain-induced crystallization at temperatures above Tg and can thereby become oriented. Following a simultaneous (SIM) biaxial strain process or a sequential (SEQ) biaxial strain process, the mechanical properties of biaxial strained tubes can be further improved. This study investigated these properties in relation to their morphology and crystal orientation. Both processes yield the same mechanical strength and modulus, yet exhibit different crystal orientation. Through further WAXS analysis it was found that the SEQ biaxial strain yields larger interplanar spacing and distorted crystals and looser packing of chains. However, this does not influence the mechanical properties negatively. A loss of orientation in SEQ biaxial strained samples at high degrees of strain was detected, but not seen for SIM biaxial strain, and did not correlate with mechanical performance in either case. However, post-annealing reduced the orientation to the same level in both cases, and the modulus and strength is decreased for both SIM and SEQ biaxial. It is therefore concluded that mechanical properties after biaxial strain are related to strain-induced amorphous orientation and the packing of crystals, rather than strain-induced crystallinity.

General information
State: Published
Organisations: Department of Micro- and Nanotechnology, Amphiphilic Polymers in Biological Sensing, Department of Energy Conversion and Storage, Imaging and Structural Analysis, Department of Wind Energy, Composites and Materials Mechanics, Mixed Conductors
Pages: 133–141
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Polymer International
Volume: 65
Issue number: 1
ISSN (Print): 0959-8103
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 0.714 SJR 0.68 CiteScore 2.2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.24 SJR 0.707 SNIP 0.777
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.732 SNIP 0.881 CiteScore 2.4
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.78 SNIP 0.962 CiteScore 2.31
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.817 SNIP 1.242 CiteScore 2.52
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.798 SNIP 1.02 CiteScore 2.09
ISI indexed (2012): ISI indexed yes
Renewable energies are a critical and necessary technological development deeply connected to human evolution and even survival. The extraordinary technological development of the past century brought tremendous changes to the planet which, despite the scepticism of some, are indubitably affecting the natural ecosystem and maybe even the destiny of Earth. Human evolution does not mean only advanced technological development, but also deeper consciousness and responsibility for the next generations to come. Everything on Earth exists because of the Sun: heat, wind, life... everything. Therefore, solar energy is one of the answers for renewable energy. In this thesis, the research has been conducted on polymer solar cells. In particular, the thesis deals with the extensive study of device lifetime, characterized with several methods: from bare benchmarking of the lifetimes, to more advanced characterizations of different device properties and materials under degradation. The devices were mostly produced using roll-to-roll processing, which is compatible with an upscaled production, essential for commercialization. Therefore, a fast characterization of a large number of samples has been a general goal of this thesis, which has been driving the choice of both the measurement techniques and also the methods for data handling. This included the development of both novel hardware and software. The possibility of fast screening a large number of devices can in fact lead to a faster improvement of the technology, due to the large amount of experimental data that would become available in a relatively short time. Real time in-situ data analysis, during the fabrication, is possibly the ultimate type of fast screening technique. In-situ X-ray diffraction analysis is a good example of a fast screening technique, that has been presented in this thesis. The challenge of standardizing the report of lifetime was addressed, with the development of novel methods for intercomparing the lifetime of a large amount of data. In particular, the comparison of the lifetime extracted under accelerated and outdoor conditions allowed for the generation of a tool for lifetime prediction. The lifetime extracted from outdoor conditions was found to be in between the one extracted from moderate conditions (shelf test and high temperature storage) and harsher conditions (light soaking and damp heat test). In-depth characterization techniques were also employed in order to study the effect of degradation on the device structure and its interfaces. This was done by exploiting different techniques that measured different properties of the device: mechanical, imaging, and electrical. Mechanical characterization of roll-to-roll processed samples allowed the detection of a mechanically weak interface between PEDOT:PSS and ZnO, which could be improved by applying a combination of humidity and high temperature. Moreover, impedance spectroscopy combined with modelling enabled identifying the degradation of the ZnO / active layer interface. Finally, imaging of cross sections of an ITO-free roll-to-roll processed device was performed successfully using transmission electron microscopy. The cross sections were prepared both with focused-ion-beam and ultramicrotomy, which gave the possibility for effectively comparing these two techniques. Moreover, the sectioning of the solar cells with a diamond blade, in the ultramicrotomy, opened the possibility...
for a fast cross sections preparation. An optimal lifetime characterization, producing relevant data for the whole OPV field, both on the macroscopic and on the microscopic level, in a fast and automatic way, is possibly the perfect lifetime characterization. The extensive characterization of lifetime performed in this thesis was done with the attempt to approach to such an optimal characterization, providing valuable results to study the effect of degradation and also providing effective tools for increasing the lifetime data exchange within the OPV research field.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Functional organic materials
Authors: Corazza, M. (Intern), Gevorgyan, S. (Intern), Krebs, F. C. (Intern)
Number of pages: 274
Publication date: 2016

Publication information
Place of publication: Riso, Roskilde
Publisher: Department of Energy Conversion and Storage, Technical University of Denmark
ISBN (Print): 978-87-92986-48-1
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
Michael_Corazza_PhD_thesis.pdf

Relations
Projects:
Publication: Research › Ph.D. thesis – Annual report year: 2016

Characterization of YBa2Cu3O7−δ Films With Various Porous Structures Grown by Metalorganic Decomposition Route
Metalorganic decomposition route with trifluoroacetates has been successfully used to fabricate YBa2Cu3O7−δ (YBCO)-based coated conductors with an excellent performance. The microstructure and superconducting properties of YBCO films were controlled by the substrate properties and the solution chemistry or by regulating the processing parameters during the film heat treatment. In this work, three YBCO films with various porous structures, namely, a fully dense sample, a cell-structured sample with dense regions surrounded by a porous structure, and a highly porous sample, were deposited on single crystalline substrates (i.e., LaAlO3 and La-doped CeO2 buffered YSZ). The samples were investigated by X-ray diffraction, scanning electron microscopy, a vibrating sample magnetometer, and a magneto-optical imaging technique. All three films show highly epitaxial growth and good superconducting properties (Tc onset around 89 K and Jc higher than 3 MA/cm2 at 77 K in self-field). However, we found that the porous structures formed by different nucleation and growth mechanisms during the sintering process still have strong influence on the superconducting properties, particularly when applying magnetic fields. The pinning behaviors in the films related to the nanoporous structures, characterized by magnetic moment measurements and visualized by magneto-optical imaging, will be discussed in detail.

General information
State: Published
Organisations: Electrofunctional materials, Department of Energy Conversion and Storage, University of Oslo
Authors: Yue, Z. (Intern), Qureishy, T. (Ekstern), Mikheenko, P. (Ekstern), Grivel, J. (Intern)
Number of pages: 4
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: IEEE Transactions on Applied Superconductivity
Volume: 26
Issue number: 3
Article number: 7200204
ISSN (Print): 1051-8223
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 1.45 SJR 0.408 SNIP 0.962
Web of Science (2017): Indexed yes
Classical molecular dynamics and quantum abs-initio studies on lithium-intercalation in interconnected hollow spherical nano-spheres of amorphous Silicon

A high concentration of lithium, corresponding to charge capacity of ~4200 mAh/g, can be intercalated in silicon. Unfortunately, due to high intercalation strain leading to fracture and consequent poor cyclability, silicon cannot be used as anode in lithium ion batteries. But recently interconnected hollow nano-spheres of amorphous silicon have been found to exhibit high cyclability. The absence of fracture upon lithiation and the high cyclability has been attributed to reduction in intercalation stress due to hollow spherical geometry of the silicon nano-particles. The present work argues that the hollow
spherical geometry alone cannot ensure the absence of fracture. Using classical molecular dynamics and density functional theory based simulations; satisfactory explanation to the absence of fracture has been explored at the atomic scale.

**General information**

State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, Defense Metallurgical Research Laboratory, Center for Study of Science, Technology and Policy, Indian Institute of Technology, Kharagpur
Authors: Bhowmik, A. (Intern), Malik, R. (Ekstern), Prakash, S. (Ekstern), Sarkar, T. (Ekstern), Bharadwaj, M. D. (Ekstern), Aich, S. (Ekstern), Ghosh, S. (Ekstern)
Number of pages: 30
Pages: 165–172
Publication date: 2016
Main Research Area: Technical/natural sciences

**Publication information**

Journal: Journal of Alloys and Compounds
Volume: 665
ISSN (Print): 0925-8388
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SJR 1.02 SNIP 1.403 CiteScore 3.66
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.05 SJR 0.954 SNIP 1.332
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.957 SNIP 1.398 CiteScore 3.03
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.117 SNIP 1.632 CiteScore 3.13
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.059 SNIP 1.583 CiteScore 2.73
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.246 SNIP 1.57 CiteScore 2.43
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.164 SNIP 1.463 CiteScore 2.41
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.073 SNIP 1.223
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.956 SNIP 1.372
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.888 SNIP 1.21
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.882 SNIP 1.209
Coatings for High Temperature Corrosion Protection of Stainless Steels

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors
Authors: Talic, B. (Intern), Molin, S. (Intern), Hendriksen, P. V. (Intern)
Number of pages: 1
Publication date: 2016
Main Research Area: Technical/natural sciences

Comparative Indoor and Outdoor Degradation of Organic Photovoltaic Cells via Inter-laboratory Collaboration

We report on the degradation of organic photovoltaic (OPV) cells to be studied at Pomona College. Power conversion efficiency and fill factor were determined from IV curves collected at regular intervals over six to eight months. Similarly prepared devices were measured indoors, outdoors, and after dark storage. Device architectures are compared. Cells kept indoors performed better than outdoors due to the lack of temperature and humidity extremes. Encapsulated cells performed better due to the minimal oxidation. Some devices showed steady aging but many failed catastrophically due to corrosion of electrodes not active device layers. Degradation of cells kept in dark storage was minimal over periods up to one year.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Functional organic materials, Pomona College, Heliatek GmbH, IMEC, Holst Center, Fraunhofer ISE, Ilmenau University of Technology, Universidad Autonoma de Barcelona
Number of pages: 8
Publication date: 2016
Main Research Area: Technical/natural sciences
Comparative study of PBI Cross Linked Utilizing Agents of Varying Steric Configurations

The high thermal and chemical stability of poly[2,2'- (m-phenylene)-5,5'-bibenzimidazole] (PBI) accounts for its wise spread use in high temperature polymer electrolyte membrane fuel cells (HT- PEMFC). By doping the membrane with phosphoric acid (PA) ionic conductivity is obtained. Thus conductivity is dependent on the amount of PA present within the membrane. However mechanical properties are reduced are significantly reduced due to the plasticizing effect shown by PA [1]. This effect is due to PBI chain displacement. This effect can be lessened by use of cross linking [2-4]. This can be obtained using ionic or covalent cross linking. When considering such, little attention is devoted to explore the effect of the sterical configuration of the cross linking agent.

In this contribution three different cross linking agents are utilized to evaluate how these affects final membrane properties.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors, Technical University of Denmark
Authors: Kirkebek, A. (Ekstern), Aili, D. (Intern), Li, Q. (Intern), Jensen, J. O. (Intern)
Pages: 124-124
Publication date: 2016

Host publication information
Title of host publication: ISPE-XV, Uppsala 15-19th August 2016
Article number: P49
Main Research Area: Technical/natural sciences
Electronic versions: Comparative_study_of_PBI_Cross_Linked_Utilizing_Agents_of_Varying_Steric_Configurations.pdf
Comparative Study of the Effect of Various Cross Linkers upon Membrane Properties

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors
Authors: Kirkebæk, A. (Intern), Alli, D. (Intern), Li, Q. (Intern), Jensen, J. O. (Intern)
Number of pages: 1
Publication date: 2016
Event: Poster session presented at Workshop on Ion Exchange Membranes for Energy Applications, Bad Zwischenahn, Germany.
Main Research Area: Technical/natural sciences
Electronic versions:
EMEA2016_Poster_Andreas_Kirkeb_k.pdf

Comparing superconducting and permanent magnets for magnetic refrigeration
We compare the cost of a high temperature superconducting (SC) tape-based solenoid with a permanent magnet (PM) Halbach cylinder for magnetic refrigeration. Assuming a five liter active magnetic regenerator volume, the price of each type of magnet is determined as a function of aspect ratio of the regenerator and desired internal magnetic field. It is shown that to produce a 1 T internal field in the regenerator a permanent magnet of hundreds of kilograms is needed or an area of superconducting tape of tens of square meters. The cost of cooling the SC solenoid is shown to be a small fraction of the cost of the SC tape. Assuming a cost of the SC tape of 6000 $/m² and a price of the permanent magnet of 100 $/kg, the superconducting solenoid is shown to be a factor of 0.3-3 times more expensive than the permanent magnet, for a desired field from 0.5-1.75 T and the geometrical aspect ratio of the regenerator. This factor decreases for increasing field strength, indicating that the superconducting solenoid could be suitable for high field, large cooling power applications.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Authors: Bjørk, R. (Intern), Nielsen, K. K. (Intern), Bahl, C. R. H. (Intern), Smith, A. (Intern), Wulff, A. C. (Intern)
Number of pages: 6
Publication date: 2016
Main Research Area: Technical/natural sciences
Comparison of the electron work function, hole concentration and exciton diffusion length for P3HT and PT prepared by thermal or acid cleavage

The electron work function, hole concentration and diffusion length were compared for poly(3-hexylthiophene) polymer (P3HT) that is commonly used for construction of solar cells, and two types of native polythiophene (PT) samples which are prospective candidates for this purpose. The polythiophene samples were prepared from 2 different precursors by thermal or chemical treatment at room temperature. Cyclic voltammetry and work function measurements were used for estimating the concentration of holes. The measured data were evaluated assuming the validity of band theory based on the tight-binding model. Published data on the valence bandwidth were used for calculating the value of the overlap integral which is related to the hole effective mass. Energy band diagrams were constructed for all 3 materials. Finally, the exciton diffusion length, which is a critical parameter for the application of conjugated polymer materials in solar cells, was measured by a modified surface photovoltage method. The approach allowed us to identify the differences in the material properties related to the processing method. Morphology of the samples determined by AFM was another tool showing these differences. It is stated that a native polythiophene prepared by treatment with acids is a prospective material for solar cells and shows a similar quality as that produced by a thermal process. © 2015 Elsevier Ltd. All rights reserved.
Comparison of ultramicrotomy and focused-ion-beam for the preparation of TEM and STEM cross section of organic solar cells

The challenge of preparing cross sections of organic photovoltaics (OPV) suitable for transmission electron microscopy (TEM) and scanning TEM (STEM) is addressed. The samples were polymer solar cells fabricated using roll-to-roll (R2R) processing methods on a flexible polyethylene terephthalate (PET) substrate. Focused ion beam (FIB) and ultramicrotomy were used to prepare the cross sections. The differences between the samples prepared by ultramicrotomy and FIB are addressed, focusing on the advantages and disadvantages of each technique. The sample prepared by ultramicrotomy yielded good resolution, enabling further studies of phase separation of P3HT:PCBM by means of energy filtered TEM (EFTEM). The sample prepared by FIB shows good structure preservation, but reduced resolution due to non-optimal thicknesses achieved after treatment. Degradation studies of samples prepared by ultramicrotomy are further discussed, which reveal particular effects of the ISOS-L-3 aging test (85 °C, 50% R.H., 0.7 Sun) onto the sample, especially pronounced in the silver layer.

General information
State: Published
Number of pages: 7
Pages: 462-468
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Applied Surface Science
Volume: 389
ISSN (Print): 0169-4332
Ratings:
Degradation, FIB, Organic photovoltaics, Phase separation, TEM, Ultramicrotomy

DOIs:
10.1016/j.apsusc.2016.07.096
Complementary analysis techniques applied on optimizing suspensions of yttria stabilized zirconia

Three different polymers with different functional groups and similar molecular weight were tested as dispersing agents for suspensions of yttria stabilized zirconia in ethanol: polyvinyl pyrrolidone, polyethylene imine, polyvinyl butyral/acetal. The stability of the system was assessed considering, in details, all the processing steps, including suspension de-agglomeration, slurry manipulation, quality of sintered tapes microstructure, and final layer leak tightness. Different analytical techniques were used to monitor ceramic de-agglomeration and stability as a function of time, for different types of dispersing agent and to optimize the dispersants concentration: Electrokinetic Sonic Amplitude was used to obtain zeta potential, Multiple Light Scattering for evaluating sedimentation rate, and multi-wavelength laser light scattering for measuring particle size distribution. All the results agree upon excellent performance of polyvinyl pyrrolidone and polyethylene imine as dispersing agents. The stability and dispersing power were finally utilized for preparing concentrated suspensions for tape casting and subsequently to sinter the tapes into dense ceramic pieces.
Complex hydrides as room-temperature solid electrolytes for rechargeable batteries

A central goal in current battery research is to increase the safety and energy density of Li-ion batteries. Electrolytes nowadays typically consist of lithium salts dissolved in organic solvents. Solid electrolytes could facilitate safer batteries with higher capacities, as they are compatible with Li-metal anodes, prevent Li dendrite formation, and eliminate risks associated with flammable organic solvents. Less than 10 years ago, LiBH$_4$ was proposed as a solid-state electrolyte. It showed a high ionic conductivity, but only at elevated temperatures. Since then a range of other complex metal hydrides has been reported to show similar characteristics. Strategies have been developed to extend the high ionic conductivity of LiBH$_4$ down to room temperature by partial anion substitution or nanoconfinement. The present paper reviews the recent developments in complex metal hydrides as solid electrolytes, discussing in detail LiBH$_4$, strategies towards fast room-temperature ionic conductors, alternative compounds, and first explorations of implementation of these electrolytes in all-solid-state batteries.

General information

State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, National Institute of Standards and Technology, Utrecht University, Tohoku University
Authors: Jongh, P. E. D. (Ekstern), Blanchard, D. (Intern), Matsuo, M. (Ekstern), Udovic, T. J. (Ekstern), Orimo, S. (Ekstern)
Number of pages: 6
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information

Volume: 122
Issue number: 3
Article number: 251
ISSN (Print): 0947-8396
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 0.699 SJR 0.481 CiteScore 1.62
Web of Science (2017): Indexed Yes
Comprehensive analysis of TEM methods for LiFePO₄/FePO₄ phase mapping: spectroscopic techniques (EFTEM, STEM-EELS) and STEM diffraction techniques (ACOM-TEM)

Transmission electron microscopy (TEM) has been used intensively in investigating battery materials, e.g. to obtain phase maps of partially (dis)charged lithium iron phosphate (LFP/FP), which is one of the most promising cathode material for next generation lithium ion (Li-ion) batteries. Due to the weak interaction between Li atoms and fast electrons, mapping of the Li distribution is not straightforward. In this work, we revisited the issue of TEM measurements of Li distribution maps for LFP/FP. Different TEM techniques, including spectroscopic techniques (energy filtered (EF)TEM in the energy range from low-loss to core loss) and a STEM diffraction technique (automated crystal orientation mapping (ACOM)), were applied to map the lithiation of the same location in the same sample. This enabled a direct comparison of the results. The maps obtained by all methods showed excellent agreement with each other. Because of the strong difference in the imaging mechanisms, it proves the reliability of both the spectroscopic and STEM diffraction phase mapping. A comprehensive comparison of all methods is given in terms of information content, dose level, acquisition time and signal quality. The latter three are crucial for the design of in situ experiments with beam sensitive Li-ion battery materials. Furthermore, we demonstrated the power of STEM diffraction (ACOM-STEM) providing additional crystallographic information, which can be analyzed to gain a deeper understanding of the LFP/FP interface properties such as statistical information on phase boundary orientation and misorientation between domains.
Conductivity and structure of sub-micrometric SrTiO$_3$-YSZ composites

Sub-micrometric composites of SrTiO$_3$-YSZ (1:1 volume) and samples of SrTiO$_3$ were prepared by high temperature consolidation of precursors obtained by precipitation with NaOH. The structure development and morphology of the precursors were studied by XRD and SEM. The perovskite and fluorite phases in the composites are clearly formed at 600°C with no signs of reaction up to 1100°C; the nominally pure SrTiO$_3$ can be formed at temperatures as low as 400°C. Composites with sub-micrometric grain sizes can be prepared successfully without reaction between the components, although a change in the cell parameter of the SrTiO$_3$ is attributed to the presence of Na. The consolidated composites were studied by impedance spectroscopy between 200 and 400°C and at a fixed temperature of 600°C with a scan in the partial pressure of oxygen. The composites did not exhibit high levels of ionic conductivity in the grain boundary nor the
bulk. The conductivity of Na-free composites shows lower levels of conductivity than pure YSZ, while samples with Na showed increased conductivity. The conductivity of SrTiO$_3$ exhibited an enhancement attributed to p-type conductivity, although contributions from protons cannot be disregarded as some Na doping is present.

**General information**

State: Published
Organisations: Department of Energy Conversion and Storage, Imaging and Structural Analysis, Fundamental Electrochemistry
Authors: Ruiz Trejo, E. (Intern), Thydén, K. T. S. (Intern), Bonanos, N. (Intern), Mogensen, M. B. (Intern)
Number of pages: 6
Pages: 82-87
Publication date: 2016
Main Research Area: Technical/natural sciences

**Publication information**

Journal: Solid State Ionics
Volume: 288
ISSN (Print): 0167-2738
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 2.64 SJR 0.856 SNIP 0.952
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.41 SJR 0.75 SNIP 0.909
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.802 SNIP 1.016 CiteScore 2.5
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.837 SNIP 1.282 CiteScore 2.62
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.903 SNIP 1.269 CiteScore 2.35
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.051 SNIP 1.253 CiteScore 2.31
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.376 SNIP 1.615 CiteScore 2.96
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.46 SNIP 1.498
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.508 SNIP 1.483
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.515 SNIP 1.617
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.292 SNIP 1.384
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.239 SNIP 1.541
Conjugated Polymers for Energy Production: Finding Suitable Candidates for Low Cost Solar Cells

This dissertation is aimed at developing materials for flexible, large area, ITO-free polymer solar cells (PSCs) fully printed under ambient conditions. A large screening of conjugated polymers, both novel and well-known materials, has been carried out in order to find suitable candidates for scalable PSCs fully printed under ambient conditions [Adv. Energy Mater. 2015, 5, 1402186]. PPDTBT resulted to be the conjugated polymer with the best photovoltaic performance within the 104 synthesized macromolecules. Therefore, further studies have been done on such material. The impact of side chain position on the physical and electrical properties of PPDTBT backbone have been evaluated, finding that anchoring a branched alkoxy chain to benzene leads to PCE as high as 3.6%, a considerably high performance for flexible ITO-free PSCs (area of approx. 1 cm²) [Macromolecules 2015, 48, 3481–3492]. Direct arylation (DAr) and direct arylation polymerization (DArP) have been applied to the preparation of PPDTBT, making this polymer readily available in only 4 synthetic steps and thus easily transferable to a large scale-production setup. DArP avoids organometallic species and therefore is an appealing polymerization method for industrial production of polymers. Several DArP protocols have been employed for the synthesis of PPDTBT leading to polymers with high structural regularity and photovoltaic performances comparable with the same materials synthesized via Stille cross-coupling polymerization. The reactivity of DArP has been further studied and applied to the synthesis of fluorinated copolymers featuring thiophene, which are largely used materials for organic electronics. In particular, by moving the bromine functionality from one monomer to the other, a big impact on the reactivity has been observed. When a thiophene-based donor monomer was brominated and copolymerized with 1,2,4,5-tetrafluorobenzene, hydrodehalogenation side reactions were suppressed, leading to the synthesis of the new PTPTPf₄ defects-free copolymer [J. Polym. Sci.Part A: Polym. Chem. 2015, 53, 2598–2605].

General information
State: Published
Organisations: Functional organic materials, Department of Energy Conversion and Storage
Authors: Livi, F. (Intern), Bundgaard, E. (Intern)
Number of pages: 251
Publication date: 2016

Publication information
Publisher: Department of Energy Conversion and Storage, Technical University of Denmark
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
Conjugated_Polymers_for_Energy_Production.pdf

Relations
Projects:
Conjugated Polymers for Energy Production
CO Oxidation on the Au$_{15}$Cu$_{15}$ Cluster and the Role of Vacancies in the MgO(100) Support

A comprehensive theoretical study of a Au$_{15}$Cu$_{15}$ cluster on MgO(100) supports and its catalytic activity for CO oxidation has been performed based on the density functional theory and microkinetic modeling. Molecular adsorption and different reaction paths based on the Langmuir–Hinshelwood (LH) and Eley–Rideal (ER) mechanisms have been explored by tuning the location of vacancies in MgO(100). The charge states of the Au$_{15}$Cu$_{15}$ cluster are negative on all supports, defect-free, O-vacancy (F-center), and Mg-vacancy (V-center), and the effect is significantly amplified on the F-center. In each case, the O$_2$ molecule can be effectively activated upon adsorption and dissociated to $2 \times$ O atoms easily, and the reaction modeling takes into account also the reaction paths with adsorbed O atoms. Overall, CO oxidation has lower reaction barriers on the cluster on the F-center. The microkinetic modeling analysis reveals that CO oxidation is very sensitive to the CO partial pressure, as the relatively strong CO binding leads readily to CO poisoning of the cluster surface sites and hinders CO$_2$ formation. For low CO partial pressures, the catalytic reaction takes place already at 150 K for the cluster on the F-center. The CO$_2$ production rates are much lower for the defect-free and V-center supports which display similar increased activity at elevated temperatures. In all cases, the right combination of CO and O$_2$ partial pressures is instrumental for CO$_2$ production.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, Aalto University, Tampere University of Technology
Authors: Ma, L. (Ekstern), Melander, M. (Intern), Weckman, T. (Ekstern), Laasonen, K. (Ekstern), Akola, J. (Ekstern)
Pages: 26747–26758
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Volume: 120
ISSN (Print): 1932-7447
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 4.58 SJR 2.135 SNIP 1.147
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.48 SJR 1.964 SNIP 1.195
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.886 SNIP 1.26 CiteScore 4.68
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.032 SNIP 1.447 CiteScore 5.08
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 2.143 SNIP 1.445 CiteScore 5.14
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.529 SNIP 1.461 CiteScore 4.98
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.339 SNIP 1.465 CiteScore 4.92
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Corrosion behavior of construction materials for ionic liquid hydrogen compressor

The corrosion behavior of various commercially available stainless steels and nickel-based alloys as possible construction materials for components which are in direct contact with one of five different ionic liquids was evaluated. The ionic liquids, namely: 1-ethyl-3-methylimidazolium triflate, 1-ethyl-3-methylimidazolium bis (trifluoromethylsulfonyl) imide, trihexyltetradecylphosphonium bis (trifluoromethylsulfonyl) imide, butyltrimethylammonium bis (trifluoromethylsulfonyl) imide, methyltrioctylammonium bis (trifluoromethylsulfonyl) imide have been identified, as performance fluids in an ionic liquid hydrogen compressor. An electrochemical cell was specially designed, and steady-state cyclic voltammetry was used to measure the corrosion resistance of the alloys in the ionic liquids at 23 °C, under atmospheric pressure. The results showed a very high corrosion resistance and high stability for all the alloys tested. The two stainless steels, AISI 316L and AISI 347 showed higher corrosion resistance compared to AISI 321 in all the ionic liquids tested. It was observed that small addition of molybdenum, tantalum, and niobium to the alloys increased the corrosion stability in the ionic liquids studied. Hastelloy® C-276 showed the poorest corrosion resistance in all the ionic liquids tested. AISI 316L with high corrosion resistance and the lowest cost is recommended as the most attractive construction material for all the components, in an ionic liquid hydrogen compressor, which are in direct contact with ionic liquids used in this study.

General information
State: Published
Organisations: Department of Mechanical Engineering, Thermal Energy, Department of Energy Conversion and Storage, Proton conductors
Authors: Arjomand Kermani, N. (Intern), Petrushina, I. (Intern), Nikiforov, A. V. (Intern), Jensen, J. O. (Intern), Rokni, M. (Intern)
Pages: 16688-16695
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Volume: 41
Issue number: 38
ISSN (Print): 0360-3199
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 4.1 SJR 1.116 SNIP 1.267
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Current Constriction at electrode/electrolyte interfaces in solid oxide cell electrochemical devices calculated via 3D reconstructions

Electrochemical devices such as batteries, fuel cells, electrolyzers, electrochemical reactors, and electrochemical sensors are important technologies for the present and the future society. For further improvement or maturing of the various technologies it is important to understand, characterize and minimize the different losses within the devices.
Decacyclene Trianhydride at Functional Interfaces: An Ideal Electron Acceptor Material for Organic Electronics

We report the interface energetics of decacyclene trianhydride (DTA) monolayers on top of two distinct model surfaces, namely, Au(111) and Ag(111). On the latter, combined valence band photoemission and X-ray absorption measurements that access the occupied and unoccupied molecular orbitals, respectively, reveal that electron transfer from substrate to surface sets in. Density functional theory calculations confirm our experimental findings and provide an understanding not only of the photoemission and X-ray absorption spectral features of this promising organic semiconductor but also of the fingerprints associated with the interface charge transfer.
Decoupling Strain and Ligand Effects in Ternary Nanoparticles for Improved ORR Electrocatalysis

Density functional theory is used to investigate OH adsorption on ternary Pt-Au-M (M = 3d-metal) nanoparticles in order to address their potential to improve activity for the oxygen reduction reaction (ORR) compared to pure Pt nanoparticles. The nanoparticles are investigated through a method developed for decoupling strain and ligand effects and then correlated with the extended Pt(111) surface for benchmarking. Subsurface Au has previously been shown to form a passivating layer, stabilising the nanoparticle catalysts against the harsh acidic conditions at the cathode, while the current study shows the effect of the ternary metal core allowing for tuning the catalytic activity through strain effects. Good agreement is found with experimental studies showing increased activity of Pt-Au-Fe/Ni nanoparticles, and the current study suggests that mid to late 3d-metals should also exhibit enhance activity and stability with respect to pure Pt nanoparticles. It is suggested that the Pt-Au-M for M = Cr, Mn, Co, Cu, Zn nanoparticles are of particular interest as they exhibit an optimal interplay between strain, ligand effects and stability.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials
Authors: C. Jennings, P. (Intern), Lysgaard, S. (Intern), Hansen, H. A. (Intern), Vegge, T. (Intern)
Number of pages: 9
Pages: 24737-24745
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Physical Chemistry Chemical Physics
Volume: 18
ISSN (Print): 1463-9076
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 4.04 SJR 1.686 SNIP 1.089
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.06 SJR 1.685 SNIP 1.113
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.725 SNIP 1.205 CiteScore 4.45
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.771 SNIP 1.239 CiteScore 4.29
Web of Science (2014): Indexed yes
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.921 SNIP 1.177 CiteScore 3.67
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.707 SNIP 1.19 CiteScore 3.6
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.817 SNIP 1.199
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.147 SNIP 1.364
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 2.166 SNIP 1.198
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.845 SNIP 1.123
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.477 SNIP 1.118
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.423 SNIP 1.1
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.191 SNIP 1.012
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.146 SNIP 0.929
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 1.634 SNIP 0.967
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 1.13 SNIP 1.115
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 0.948 SNIP 1.079
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 0.121 SNIP 0
Original language: English
Electronic versions:
Decoupling Strain and Ligand Effects in Ternary Nanoparticles for Improved ORR Electrocatalysis.pdf
DOIs:
10.1039/C6CP04194A

Bibliographical note
Degradation of solid oxide cells during co-electrolysis of steam and carbon dioxide at high current densities

In this work, the durability of Ni–YSZ based solid oxide cells was investigated during co-electrolysis of steam and carbon dioxide (45% H₂O + 45% CO₂ + 10% H₂) at current density of −1.5 or −2.0 A cm⁻². The cell consists of ∼300 μm Ni–YSZ support, ∼10 μm Ni–YSZ electrode, ∼10 μm YSZ electrolyte and ∼15 μm LSM–YSZ oxygen electrode. The gas conversion was 45% at −1.5 A cm⁻² and 60% at −2.0 A cm⁻², and the operating durations were up to 700 h. The detailed electrochemical analysis revealed significant increase of the ohmic resistance, oxide ion transport resistance in the Ni–YSZ composite electrodes and the electrochemical reaction resistance at the Ni–YSZ triple-phase boundaries. The performance degradation is mainly ascribed to the microstructural change in the Ni–YSZ electrode close to the YSZ electrolyte, including the percolation loss of Ni, the contact loss between Ni and YSZ electrolyte and the decomposition of YSZ close to Ni–YSZ|YSZ interface. The electrochemical performance and the microstructure of the oxygen electrode were found to be relatively stable.
Descriptors and Thermodynamic Limitations of Electrocatalytic Carbon Dioxide Reduction on Rutile Oxide Surfaces

A detailed understanding of the electrochemical reduction of CO₂ into liquid fuels on rutile metal oxide surfaces is developed by using DFT calculations. We consider oxide overlayer structures on RuO₂(1 1 0) surfaces as model catalysts to elucidate the trends and limitations in the CO₂ reduction reaction (CO₂RR) based on thermodynamic analysis. We aim to specify the requirements for CO₂RR catalysts to establish adsorbate scaling relations and use these to derive activity volcanoes. Computational results show that the OH* binding free energy is a good descriptor of the thermodynamic limitations and it defines the left leg of the activity volcano for CO₂RR. HCOOH* is a key intermediate for products formed through further reduction, for example, methanediol, methanol, and methane. The surfaces that do not bind HCOOH* are selective towards formic acid (HCOOH) production, but hydrogen evolution limits their suitability. We determine the ideal binding free energy for H* and OH* to facilitate selective CO₂RR over H₂/CO evolution to be ΔG₂[H]>0.5 eV and ~0.5
eV<ΔG_{R[OH]}<0.1 eV. The Re-containing overlayers considered in this work display excellent promise for selectivity, although they are active at a highly reducing potential.

**General information**

*State:* Published

*Organisations:* Department of Energy Conversion and Storage, Atomic scale modelling and materials

*Authors:* Bhowmik, A. (Intern), Vegge, T. (Intern), Hansen, H. A. (Intern)

*Number of pages:* 15

*Pages:* 3230–3243

*Publication date:* 2016

*Main Research Area:* Technical/natural sciences

**Publication information**

*Journal:* ChemSusChem

*Volume:* 9

*Issue number:* 22

*ISSN (Print):* 1864-5631

*Ratings:*

- BFI (2018): BFI-level 2
- Web of Science (2018): Indexed yes
- BFI (2017): BFI-level 1
- Scopus rating (2017): CiteScore 6.86 SJR 2.538 SNIP 1.235
- Web of Science (2017): Indexed Yes
- BFI (2016): BFI-level 1
- Scopus rating (2016): CiteScore 6.7 SJR 2.505 SNIP 1.311
- Web of Science (2016): Indexed yes
- BFI (2015): BFI-level 1
- Scopus rating (2015): SJR 2.53 SNIP 1.424 CiteScore 7.33
- Web of Science (2015): Indexed yes
- BFI (2014): BFI-level 1
- Scopus rating (2014): SJR 2.864 SNIP 1.663 CiteScore 7.97
- Web of Science (2014): Indexed yes
- BFI (2013): BFI-level 1
- Scopus rating (2013): SJR 2.561 SNIP 1.46 CiteScore 6.79
- ISI indexed (2013): ISI indexed yes
- Web of Science (2013): Indexed yes
- Scopus rating (2012): SJR 3.054 SNIP 1.553 CiteScore 6.72
- ISI indexed (2012): ISI indexed yes
- Scopus rating (2011): SJR 2.759 SNIP 1.497 CiteScore 5.53
- ISI indexed (2011): ISI indexed no
- Web of Science (2011): Indexed yes
- Scopus rating (2010): SJR 1.959 SNIP 1.143
- Web of Science (2010): Indexed yes
- Scopus rating (2009): SJR 0.979 SNIP 0.718
- BFI (2008): BFI-level 1
- Scopus rating (2008): SJR 0.297 SNIP 0.508
- Web of Science (2008): Indexed yes
- Scopus rating (2007): SJR 0.281 SNIP 0.49
- Scopus rating (2006): SJR 0.242 SNIP 0.37
- Scopus rating (2005): SJR 0.195 SNIP 0.287
- Scopus rating (2004): SJR 0.214 SNIP 0.272
- Scopus rating (2003): SJR 0.276 SNIP 0.417
- Scopus rating (2002): SJR 0.3 SNIP 0.584
- Scopus rating (2001): SJR 0.29 SNIP 0.496
- Scopus rating (2000): SJR 0.425 SNIP 0.571
- Scopus rating (1999): SJR 0.5 SNIP 0.688

*Original language:* English
Design and optimization of porous ceramic supports for asymmetric ceria-based oxygen transport membranes

The microstructure, mechanical properties and gas permeability of porous supports of Ce$_{0.9}$Gd$_{0.1}$O$_{1.95-δ}$ (CGO) were investigated as a function of sintering temperature and volume fraction of pore former for use in planar asymmetric oxygen transport membranes (OTMs). With increasing the pore former content from 11 vol% to 16 vol%, the gas permeabilities increased by a factor of 5 when support tapes were sintered to comparable densities. The improved permeabilities were due to a more favourable microstructure with larger interconnected pores at a porosity of 45% and a fracture strength of 47±2 MPa (m=7). The achieved gas permeability of $2.25 \times 10^{-15}$ m$^2$ for a 0.4 mm thick support will not limit the gas transport for oxygen production but in partial oxidation of methane to syngas at higher oxygen fluxes. For integration of the CGO support layer into a flat, asymmetric CGO membrane, the sintering activity of the CGO membrane was reduced by Fe$_2$O$_3$ addition (replacing Co$_3$O$_4$ as sintering additive).
Determination of Water Vapor Pressure Over Corrosive Chemicals Versus Temperature Using Raman Spectroscopy as Exemplified with 85.5% Phosphoric Acid

A method to determine the water vapor pressure over a corrosive substance was developed and tested with 85.5±0.4% phosphoric acid. The water vapor pressure was obtained at a range of temperatures from ∼25°C to ∼200°C using Raman spectrometry. The acid was placed in an ampoule and sealed with a reference gas (either hydrogen or methane) at a known pressure (typically ∼0.5 bar). By comparing the Raman signals from the water vapor and the references, the water pressure was determined as a function of temperature. A considerable amount of data on the vapor pressure of phosphoric acid are available in the literature, to which our results could successfully be compared. A record value of the vapor pressure, 3.40 bar, was determined at 210°C. The method required a determination of the precise Raman scattering ratios between the substance, water, and the used reference gas, hydrogen or methane. In our case the scattering ratios between water and reference ν₁ Q-branches were found to be 1.20±0.03 and 0.40±0.02 for H₂ and CH₄, respectively.
Corrosive substance, Raman, Gas phase, Phosphoric acid, Scattering cross-section, Vapor pressure
Development of a novel rotary magnetic refrigerator

A novel rotary magnetic refrigerator was designed and built at the Federal University of Santa Catarina (UFSC). The optimized magnetic circuit is a two-pole system in a rotor-stator configuration with high flux density regions of approximately 1 T. Eight pairs of stationary regenerator beds filled with approximately 1.7 kg of gadolinium spheres (425-600 μm diameter) were placed in the magnetic gap. Two low-friction rotary valves were developed to synchronize the hydraulic and magnetic cycles. The valves were positioned at the hot end to avoid heat generation in the cold end. In this work, experimental results are presented as a function of the operating frequency, fluid flow rate, hot reservoir temperature and thermal load. The performance of the device was evaluated in terms of the coefficient of performance (COP) and overall second-law efficiency ($\eta_{2nd}$). The maximum no-load temperature span was 12 K at 1.5 Hz and 150 L h$^{-1}$, and the maximum zero-span cooling power was 150 W at 0.8 Hz and 200 L h$^{-1}$. For a thermal load of 80.4 W, at 0.8 Hz and 200 L h$^{-1}$, the device generated a temperature span of 7.1 K, with a COP of 0.54 and $\eta_{2nd}$ of 1.16%.

General information

State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Federal University of Santa Catarina
Authors: Lozano, J. A. (Ekstern), Capovilla, M. S. (Ekstern), Trevizoli, P. V. (Ekstern), Engelbrecht, K. (Intern), Bahl, C. (Intern), Barbosa, J. R. (Ekstern)
Number of pages: 11
Pages: 187-197
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information

Journal: International Journal of Refrigeration
Volume: 68
ISSN (Print): 0140-7007
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 1.888 SJR 1.471 CiteScore 3.46
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.06 SJR 1.371 SNIP 1.607
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.349 SNIP 1.532 CiteScore 2.44
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.619 SNIP 2.086 CiteScore 2.6
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.422 SNIP 1.944 CiteScore 2.25
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.386 SNIP 1.893 CiteScore 2.09
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
Dry Etching

Production of large-area flat panel displays (FPDs) involves several pattern transfer and device fabrication steps that can be performed with dry etching technologies. Even though the dry etching using capacitively coupled plasma is generally used to maintain high etch uniformity, due to the need for the higher processing rates in FPDs, high-density plasma processing tools that can handle larger-area substrate uniformly are more intensively studied especially for the dry etching of polysilicon thin films. In the case of FPD processing, the current substrate size ranges from 730 × 920 mm (fourth generation) to 2,200 × 2,500 mm (eighth generation), and the substrate size is expected to increase further within a few years. This chapter aims to present relevant details on dry etching including the phenomenology, materials to be etched with the different recipes, plasma sources fulfilling the dry etching requirements, and advantages of dry etching over wet processing. Current status and future trends are also presented.

General information

State: Published
Organisations: Electrofunctional materials, Fundamental Electrochemistry, Department of Energy Conversion and Storage, Sungkyunkwan University
Authors: Stamate, E. (Intern), Yeom, G. Y. (Ekstern)
Pages: 1343-1356
Publication date: 2016

Host publication information

Title of host publication: Handbook of Visual Display Technology
Publisher: Springer
Editors: Chen, J., Cranton, W., Fihn, M.
Edition: 2
ISBN (Print): 978-3-319-14345-3, 978-3-319-14347-7
ISBN (Electronic): 978-3-319-14346-0
Main Research Area: Technical/natural sciences
Durability Issues and Status of HT-PEM Based on Acid Doped Polybenzimidazoles

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors, Technical University of Denmark
Authors: Jensen, J. O. (Intern), Cleemann, L. N. (Intern), Li, Q. (Intern), Jakobsen, M. T. D. (Ekstern)
Number of pages: 1
Publication date: 2016
Event: Abstract from Hydrogen Day 2016, Prague, Czech Republic.
Main Research Area: Technical/natural sciences
Electronic versions:
Abstract_CISTEM_Symposium_6_8_April_2016_Prague.pdf
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2017

Durability Issues and Status of PBI-Based Fuel Cells
This chapter briefly reviews durability and stability issues with key materials and components for HT-PEMFCs, including the polymer membrane, the doping acid, the electrocatalyst, the catalyst support and bipolar plates. Degradation mechanisms and their dependence on fuel cell operating conditions are summarized as well. To date, lifetimes of this type of fuel cells of up to 18,000 h with degradation rates of around 5 μV/h at temperatures of 150–160 °C have been demonstrated using hydrogen and air under constant moderate load. However, the degradation rate increases by a factor 10 when the cell is exposed to start-up–shutdown or load cycling.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors
Authors: Jakobsen, M. T. D. (Intern), Jensen, J. O. (Intern), Cleemann, L. N. (Intern), Li, Q. (Intern)
Number of pages: 23
Pages: 487-509
Publication date: 2016

Host publication information
Title of host publication: High Temperature Polymer Electrolyte Membrane Fuel Cells: Approaches, Status, and Perspectives
Place of publication: Switzerland
Publisher: Springer
Editors: Li, Q., Aili, D., Hjuler, H. A., Jensen, J. O.
ISBN (Print): 978-3-319-17081-7
ISBN (Electronic): 978-3-319-17082-4
Chapter: 22
Main Research Area: Technical/natural sciences
DOIs:
10.1007/978-3-319-17082-4_22
Source: Findit
Source-ID: 2187916955
Publication: Research - peer-review › Book chapter – Annual report year: 2015

Ecodesign perspectives of thin-film photovoltaic technologies: A review of life cycle assessment studies
Here, we review 33 life cycle assessment (LCA) studies of thin-film photovoltaic (PV) technologies that have had a holistic coverage in their assessments and/or have included ecodesign aspects. Only five of them were found to have a comprehensive life cycle and impact coverage, and their analyses highlighted the importance of (i) including the entire life cycle of the PV system, in particular the often-omitted disposal stage, and (ii) assessing all relevant impact categories and not just climate change or energy requirements to minimise the risk of burden-shifting. Out of the 28 studies embracing ecodesign considerations in parts of the PV life cycle, the analysis of the eleven of them addressing primary energy demand during module production suggests that electricity consumption during the metal deposition processes is a top contributor and should be prioritised by PV technology developers. A similar analysis of the ten studies having included the balance of system components (BOS) in the assessments showed that these contribute significantly to most environmental impact categories. Beyond recommending that stakeholders in the PV field rely on LCA to support decision-making and to guide scientific research and technological development, we strongly advocate LCA practitioners to include
the entire PV system, including the BOS, to identify ecodesign opportunities without risking potential burden-shifting across the different parts of the system and across impact categories.
Economic feasibility of CHP facilities fueled by biomass from unused agriculture land: Case of Croatia

In this paper, the energy potential of biomass from growing short rotation coppice on unused agricultural land in the Republic of Croatia is used to investigate the feasibility of Combined Heat and Power (CHP) facilities fueled by such biomass. Large areas of agricultural land that remain unused for food crops, represent significant potential for growing biomass that could be used for energy. This biomass could be used to supply power plants of up to 15MWe in accordance with heat demands of the chosen locations. The methodology for regional energy potential assessment was elaborated in previous work and is now used to investigate the conditions in which such energy facilities could be feasible. The overall potential of biomass from short rotation coppice cultivated on unused agricultural land in the scenarios with 30% of the area is up to 10PJ/year. The added value of fruit trees pruning biomass represents an incentive for the development of fruit production on such agricultural land. Sensitivity analysis was conducted for several parameters: cost of biomass, investment costs in CHP systems and combined change in biomass and technology cost.
Economic feasibility of CHP facilities fuelled by biomass from unused agriculture land_case of Croatia.postprint. Embargo ended: 02/05/2018

DOIs: 10.1016/j.enconman.2016.04.090

Source: FindIt
Source-ID: 2304051425
Publication: Research - peer-review › Journal article – Annual report year: 2016

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science
Authors: Esposito, V. (Intern)
Number of pages: 1
Publication date: 2016
Main Research Area: Technical/natural sciences
Editorial for the special issue life cycle, environmental, ecology and impact analysis of solar technology

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Functional organic materials, Technical University of Cartagena, Star Science
Authors: Espinosa, N. (Ekstern), Krebs, F. C. (Intern), Lampert, C. M. (Ekstern)
Number of pages: 1
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Volume: 156
ISSN (Print): 0927-0248
Ratings:

BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes

BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 4.83 SJR 1.459 SNIP 1.532
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.97 SJR 1.599 SNIP 1.71
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.8 SNIP 1.851 CiteScore 5.16
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.19 SNIP 2.348 CiteScore 5.87
Web of Science (2014): Indexed yes
The effect of some platinum group metals (PGM = Rh, Pd, and Pt) on the microstructure and critical current density of Cu/Nb-sheathed MgB2 wires has been studied using Mg$_{1-x}$PGM$_x$B$_2$ powders with low doping levels. It was found that Pt and Pd do not enter the MgB2 lattice and have only limited influence on Tc. In contrast, some Rh can be substituted and induces a decrease of Tc. Secondary phases are formed when the solubility limit is exceeded, but they have different morphologies depending on the dopant. For some of these PGM elements, flux pinning improvements have been observed at low fields. The results are discussed in comparison with previous investigations using other transition metals for doping on the Mg site.

**General information**

State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Ecosystems Programme, University of Barcelona
Authors: Grivel, J. (Intern), Alexiou, A. (Intern), Namazkar, S. (Intern), Pitillas, A. (Ekstern)
Number of pages: 5
Effect of pore formers on properties of tape cast porous sheets for electrochemical flue gas purification

Ce0.9Gd0.1O1.95 (CGO) electrolytes for electrochemical flue gas purification multilayers were fabricated by tape casting and sintering using different types, shapes and sizes of pore formers. The resulting tapes (with thickness of about 400μm) were characterized by scanning electron microscopy, gas permeability measurements, mercury porosimetry and pore orientation measurements, to investigate the role of the different pore formers on the properties after sintering at a temperature of 1250°C. Those tapes prepared from different non-spherical pore formers with comparable porosity of about 43%, showed significant differences in gas permeability which could be correlated to an increase in mean pore size and pore connectivity. The degree of pore orientation in the tape casting direction was determined by best-fit ellipse method and a modified linear intercept method and the obtained data were correlated with the corresponding gas permeability.
Effect of substrate curvature on Mn-Co-O spinel coatings prepared by electrophoretic deposition for solid oxide fuel cells

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Mixed Conductors, Ceramic Engineering & Science
Authors: Wulff, A. C. (Intern), Molin, S. (Intern), Andersen, K. B. (Intern), Zielke, P. (Intern), Frandsen, H. L. (Intern)
Number of pages: 1
Publication date: 2016
Main Research Area: Technical/natural sciences
Links:
http://www.sustain.dtu.dk/

Bibliographical note
Sustain Abstract M-11
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2016

Effects of current stress and thermal storage on polymeric heterojunction P3HT:PCBM solar cell
We subjected P3HT:PCBM solar cells to electrical constant current stress and thermal storage. We employed the impedance spectroscopy technique combined to conventional DC measurements for device characterization during all stresses. We identified and separated different contributions affecting the open circuit voltage and short circuit current. Several mechanisms are behind these changes during the stresses; in particular, we underlined the exciton recombination rate and the variation of the built-in voltage.

General information
Effects of flow balancing on active magnetic regenerator performance

Experiments with a recently constructed rotary multi-bed active magnetic regenerator (AMR) prototype have revealed strong impacts on the temperature span from variations in the resistances of the flow channels carrying heat transfer fluid in and out of the regenerator beds. In this paper we show through numerical modeling how unbalanced flow in the beds decreases the cooling power and COP for a dual bed device. Furthermore, it is shown how resistance variations in multi-bed devices give rise to unbalanced flow in the individual beds and how this decreases cooling powers and COPs of the machines by approximately 30% and 50%, respectively.

General information

State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Authors: Eriksen, D. (Intern), Engelbrecht, K. (Intern), Bahl, C. (Intern), Bjørk, R. (Intern), Nielsen, K. K. (Intern)
Number of pages: 8
Pages: 1-8
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Applied Thermal Engineering
Volume: 103
ISSN (Print): 1359-4311
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 4.14 SJR 1.505 SNIP 1.837
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.78 SJR 1.438 SNIP 1.851
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.683 SNIP 1.884 CiteScore 3.32
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.539 SNIP 2.187 CiteScore 3.16
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Bismuth antimony telluride (Bi$_x$Sb$_{2-x}$Te$_3$, 0.4 <x<0.6) is one of the best and most-used p-type semiconductor materials for near-room-temperature thermoelectric power generation. In this work, p-type Bi$_{0.4}$Sb$_{1.6}$Te$_3$ samples were prepared under various conditions (temperature, holding time, and ramp-rate) using spark plasma sintering (SPS). The effects of SPS conditions on the anisotropic thermoelectric properties and microstructure evolutions were systematically investigated. The change of sintering temperature showed stronger influence than other sintering parameters to the resulting thermoelectric properties. Samples sintered over the temperature range between 653 K and 773 K showed significant differences in the degrees of orientations. The change was mainly caused by grain growth and re-orientation.

Despite of the anisotropy, zT value as high as 1.2 to 1.3 was achieved over the temperature range of 300 to 360 K by directly using commercial power sintered at 723 and 773 K. The sintering profiles and microstructure evolutions during SPS were illustrated and the thermoelectric properties as a function of the degrees of orientations were shown and discussed in detail.
Long-term strong cathodic polarization experiments of down to -2.4 V vs. $E^\circ(O_2)$ of the Ni-YSZ interface were performed at 900°C in 97% H$_2$/3% H$_2$O on model electrodes. The Ni-YSZ interface underwent extensive changes and a large affected volume with a complex microstructure and phase distribution resulted. Impedance spectroscopy shows initial decrease but later increase in the series resistance and polarization resistance during the 140-160 h of polarization, and significant inductive behavior. An intermetallic Ni-Zr phase that formed during polarization was preserved when the polarization was kept during cooling, and was identified post-mortem by transmission electron microscopy as Ni$_7$Zr$_2$. ZrO$_2$ nanoparticles were formed on the Ni-gas surface next to the Ni-YSZ-gas triple phase boundary. Explanations of the observed features are offered based on electron microscopy and impedance spectroscopy.
Main Research Area: Technical/natural sciences

**Publication information**
Journal: Electrochemical Society. Journal
Volume: 163
Issue number: 10
ISSN (Print): 0013-4651

**Ratings:**
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 3.48 SJR 1.267 SNIP 1.009
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.97 SJR 1.222 SNIP 0.963
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.115 SNIP 1.066 CiteScore 3.17
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.213 SNIP 1.25 CiteScore 3.36
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.169 SNIP 1.309 CiteScore 2.92
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.329 SNIP 1.281 CiteScore 2.61
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.331 SNIP 1.335 CiteScore 2.74
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.418 SNIP 1.304
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.442 SNIP 1.27
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.595 SNIP 1.41
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.569 SNIP 1.322
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.608 SNIP 1.535
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.523 SNIP 1.481
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.712 SNIP 1.7
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.971 SNIP 1.677
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 2.036 SNIP 1.618
Web of Science (2002): Indexed yes
Effects of surface finish and mechanical training on Ni-Ti sheets for elastocaloric cooling

Elastocaloric cooling has emerged as a promising alternative to vapor compression in recent years. Although the technology has the potential to be more efficient than current technologies, there are many technical challenges that must be overcome to realize devices with high performance and acceptable durability. We study the effects of surface finish and training techniques on dog bone shaped polycrystalline samples of NiTi. The fatigue life of several samples with four different surface finishes was measured and it was shown that a smooth surface, especially at the edges, greatly improved fatigue life. The effects of training both on the structure of the materials and the thermal response to an applied strain was studied. The load profile for the first few cycles was shown to change the thermal response to strain, the structure of the material at failure while the final structure of the material was weakly influenced by the surface finish.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Department of Wind Energy, Materials science and characterization
Number of pages: 6
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: A P L Materials
Volume: 4
Article number: 064110
ISSN (Print): 2166-532X
Ratings:
Web of Science (2018): Indexed yes
Scopus rating (2017): CiteScore 3.78 SJR 1.63 SNIP 0.942
Web of Science (2017): Indexed Yes
Scopus rating (2016): SJR 2.177 SNIP 1.151 CiteScore 3.67
Web of Science (2016): Indexed yes
Scopus rating (2015): SJR 2.081 SNIP 1.236 CiteScore 3.76
Scopus rating (2014): SJR 1.628 SNIP 1.195 CiteScore 2.9
Original language: English
Shape memory effect, Surface finishing, Stress strain relations, Materials modification, Testing procedures
Electronic versions:
Effects_of_surface_finish_and_mechanical_training_on_Ni_Ti_sheets_for_elastocaloric_cooling.pdf
DOIs:
10.1063/1.4955131

Bibliographical note
All article content, except where otherwise noted, is licensed under a Creative Commons Attribution (CC BY) license (http://creativecommons.org/licenses/by/4.0/)
Publication: Research - peer-review › Journal article – Annual report year: 2016
Efficient modeling of metallic interconnects for thermo-mechanical simulation of SOFC stacks: homogenized behaviors and effect of contact

Currently thermo-mechanical analysis of the entire solid oxide fuel cell (SOFC) stack at operational conditions is computationally challenging if the geometry of metallic interconnects is considered explicitly. This is particularly the case when creep deformations in the interconnect are considered in addition to elasticity. In this work, this problem is addressed using homogenization, whereby the effect of the geometry is built into an effective anisotropic material law for a continuum block of material, which then represents the interconnect in the stack model. The study presents a finite element model to calculate the homogenized mechanical response of corrugated metallic interconnects at high temperatures. Thereafter, a constitutive law for the homogenized structure (effective material law) is developed. In order to properly describe the mechanical behavior of the interconnect at high temperature, deformations involving the elastic, creep as well as effect of changes in the geometry due to contact should be accounted for. The constitutive law can be applied using 3D modeling, but for simple presentation of the theory, 2D plane strain formulation is used to model the corrugated metallic interconnect. Finally, the developed constitutive law is verified by comparing its predictions for creep strain with results from the original 2D finite element model for different loading conditions. The constitutive law is found to satisfactorily describe the mechanical behavior of corrugated metallic interconnect with computational feasibility and significant speed gain.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors
Authors: Tadesse Molla, T. (Intern), Kwok, K. (Intern), Frandsen, H. L. (Intern)
Number of pages: 12
Pages: 6433-6444
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Volume: 41
ISSN (Print): 0360-3199
Ratings:
  BFI (2018): BFI-level 1
  Web of Science (2018): Indexed yes
  BFI (2017): BFI-level 2
  Scopus rating (2017): CiteScore 4.1 SJR 1.116 SNIP 1.267
  Web of Science (2017): Indexed yes
  BFI (2016): BFI-level 2
  Scopus rating (2016): CiteScore 3.74 SJR 1.145 SNIP 1.315
  Web of Science (2016): Indexed yes
  BFI (2015): BFI-level 2
  Scopus rating (2015): SJR 1.27 SNIP 1.314 CiteScore 3.46
  Web of Science (2015): Indexed yes
  BFI (2014): BFI-level 2
  Scopus rating (2014): SJR 1.207 SNIP 1.484 CiteScore 3.54
  Web of Science (2014): Indexed yes
  BFI (2013): BFI-level 2
  Scopus rating (2013): SJR 1.265 SNIP 1.449 CiteScore 3.38
  ISI indexed (2013): ISI indexed yes
  Web of Science (2013): Indexed yes
  BFI (2012): BFI-level 2
  Scopus rating (2012): SJR 1.499 SNIP 1.708 CiteScore 3.96
  ISI indexed (2012): ISI indexed yes
  Web of Science (2012): Indexed yes
  BFI (2011): BFI-level 2
  Scopus rating (2011): SJR 1.443 SNIP 1.828 CiteScore 4.42
  ISI indexed (2011): ISI indexed yes
  Web of Science (2011): Indexed yes
  BFI (2010): BFI-level 2
  Scopus rating (2010): SJR 1.579 SNIP 1.854
Elastic Properties of the Solid Electrolyte Li$_7$La$_3$Zr$_2$O$_{12}$ (LLZO)

The oxide known as LLZO, with nominal composition Li$_7$La$_3$Zr$_2$O$_{12}$, is a promising solid electrolyte for Li-based batteries due to its high Li ion conductivity and chemical stability with respect to lithium. Solid electrolytes may also enable the use of metallic Li anodes by serving as a physical barrier that suppresses dendrite initiation and propagation during cycling. Prior linear elasticity models of the Li electrode/solid electrolyte interface suggest that the stability of this interface is highly dependent on the elastic properties of the solid separator. For example, dendritic suppression is predicted to be enhanced as the electrolyte’s shear modulus increases. In the present study a combination of first-principles calculations, acoustic impulse excitation measurements, and nanoindentation experiments are used to determine the elastic constants and moduli for high-conductivity LLZO compositions based on Al and Ta-doping. The calculated and measured isotropic shear modulus are in good agreement, and fall within the range of 56 to 61 GPa. These values are an order of magnitude larger than for Li metal, and far exceed the minimum value (~8.5 GPa) believed to be necessary to suppress dendrite initiation. These data suggest that LLZO exhibits sufficient stiffness to warrant additional development as a solid electrolyte for Li batteries.
The aim of this article is to analyze the elastocaloric effect of a commercial Ni-Ti plate for its application in a cooling device. In the first part, the article shows numerical results of the cooling characteristics of a regenerator-based elastocaloric cooling device with different thickness of the Ni-Ti plates based on a previously developed numerical model. It is shown that such a device (with a plate thickness of 0.1 mm) can produce a specific cooling power up to 7 kW/kg and coefficient of performance values up to 5 at the 30 K of the temperature span. In the second part of the article, a testing and analysis of the elastocaloric effect of the Ni-Ti plate using infrared thermography is shown. Prior to the elastocaloric testing, the sample was mechanically polished and subjected to 200 loading–unloading cycles at a slow strain-rate and 10,000 loading–unloading cycles at high strain-rate to stabilize its superelastic behavior and evaluate its fatigue life. When the functional and structural stability was reached and relatively good fatigue resistance was proven, the elastocaloric effect of the sample was studied with an infrared camera as a function of strain-rate and applied strain. It is shown that the adiabatic conditions are well approximated at strain-rates above 0.1 s⁻¹. The largest adiabatic temperature change of 14 K during loading and 12.5 K during unloading were measured at the applied strain of 4.2% (at a strain-rate of 0.33 s⁻¹). The homogeneity of the elastocaloric effect and the temperature irreversibilities during unloading are presented and discussed. It can be concluded that thin Ni-Ti plates with suitable austenitic finish temperature are good candidates to be applied in a proof-of-concept regenerator-based cooling device.
Electric field control of the $\gamma$-Al$_2$O$_3$/SrTiO$_3$ interface conductivity at room temperature

Controlling interfaces using electric fields is at the heart of modern electronics. The discovery of the conducting interface between the two insulating oxides LaAlO$_3$ (LAO) and SrTiO$_3$ (STO) has led to a number of interesting electric field-dependent phenomena. Recently, it was shown that replacing LAO with a spinel $\gamma$-Al$_2$O$_3$ (GAO) allows a good pseudo-epitaxial film growth and high electron mobility at low temperatures. Here, we show that the GAO/STO interface resistance, similar to LAO/STO, can be tuned by orders of magnitude at room temperature using the electric field of a backgate. The resistance change is non-volatile, bipolar, and can be tuned continuously rather than being a simple on/off switch. Exposure to light significantly changes the capabilities to tune the interface resistance. High- and low-resistive states are obtained by annihilation and creation, respectively, of free $n$-type carriers, and we speculate that electromigration of oxygen vacancies is the origin of the tunability.

General information

State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, University of Copenhagen
Number of pages: 4
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Volume: 109
Issue number: 2
Article number: 021602
ISSN (Print): 0003-6951

Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 3.25 SJR 1.382 SNIP 1.167
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.67 SJR 1.673 SNIP 1.249
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.499 SNIP 1.226 CiteScore 2.47
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.861 SNIP 1.492 CiteScore 3.25
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.146 SNIP 1.633 CiteScore 3.77
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 2.57 SNIP 1.739 CiteScore 3.76
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 2.814 SNIP 1.917 CiteScore 4.04
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 2.92 SNIP 1.775
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.826 SNIP 1.834
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 2.894 SNIP 1.82
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 3.012 SNIP 1.916
Web of Science (2007): Indexed yes
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 3.755 SNIP 2.353
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 3.992 SNIP 2.367
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 3.897 SNIP 2.275
Web of Science (2003): Indexed yes
Electrochemical Characterization of PEMECs Operating at Various Current Densities

This conference contribution touches upon electrochemical characterization of operating polymer electrolyte membrane electrolysis cells (PEMECs) by the application of electrochemical impedance spectroscopy (EIS). Analysis of differences in impedance spectra (ADIS) (Jensen et al., 2007) can be applied to gain insight into the relative magnitudes of resistance contributions from the two electrodes, the electrolyte and of mass transfer limitations and can help identifying the time scale of the respective processes. The gained knowledge may facilitate further development of the PEMECs.

General information
State: Published
Authors: Elsøe, K. (Intern), G.-Madsen, L. (Ekstern), Scherer, G. G. (Ekstern), Hjelm, J. (Intern), Mogensen, M. B. (Intern)
Publication date: 2016
Conference: PRiME 2016/230th ECS Meeting, Honolulu, United States, 02/10/2016 - 02/10/2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Electrochemical Society. Meeting Abstracts (Online)
Volume: MA2016-02
Issue number: 38
Article number: 2408
ISSN (Print): 2151-2043
Original language: English
Links:
http://ma.ecsdl.org/content/MA2016-02/38/2408.abstract?sid=f6e5ab15-e4a2-45ba-82f8-177f51791c37
Source: FindIt
Source-ID: 2344805999
Publication: Research - peer-review › Conference abstract in journal – Annual report year: 2016

Electrochemical Impedance Spectroscopy on Industrially-Relevant Solid Oxide Electrolyzer Cell Stacks: A Powerful Tool for In-Situ Investigations of Degradation Mechanisms

In the current efforts of moving energy production to renewable sources, wind and solar energy are widely considered as the key technologies to cover our growing demands. However, the fluctuating nature of these sources requires a flexible energy system and storage technologies to ensure that energy services can be covered in a stable and affordable manner. One promising solution is the synthetic fuel production by solid oxide electrolyzers. Electricity can be stored in a power-to-gas process during times of excess electricity production and then further converted to liquid fuels for e.g. transportation, or at high demands converted back to electricity by either conventional power plants or fuel cells.

One of today's biggest hurdles for a successful commercialization of solid oxide electrolyzers is the stack's lifetime with current industry targets in the order of five to ten years. To identify and quantify the different degradation mechanisms sensitive in-situ analysis tools are needed. On single cell level, electrochemical impedance spectroscopy (EIS) is a well-established diagnostics tool. On stack level EIS has been shown to be more difficult because of geometrical restrictions of the stack design and significantly lower resistances due to the larger active cell area. Nevertheless, it is becoming a more and more important technique for stack diagnostics.

Here we present impedance spectroscopy results of two solid oxide stacks provided by Haldor Topsoe A/S. The first stack was a 14-cell stack (Delta design) specifically optimized for EIS measurements, while the other stack was an 8-cell stack (TSP-1 design), where impedance measurements were carried out without major modifications to the stack. The individual cell voltages were monitored simultaneously by EIS during up to 2000 hours in electrolysis within the ForskEL project
2015-1-12276 "Towards Solid Oxide Electrolysis Plants in 2020", funded by Danish Energet.dk. The analysis provides valuable insight into the degradation processes which could not have been obtained by current-voltage-data alone.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Applied Electrochemistry, Haldor Topsoe AS
Authors: Zielke, P. (Intern), Høgh, J. V. T. (Intern), Chen, M. (Intern), Kiebach, W. (Intern), Küngas, R. (Ekstern), Blennow, P. (Ekstern), Hjelm, J. (Intern), Hendriksen, P. V. (Intern)
Publication date: 2016
Conference: PRIME 2016/230th ECS Meeting, Honolulu, United States, 02/10/2016 - 02/10/2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Electrochemical Society. Meeting Abstracts (Online)
Volume: MA2016-02
Article number: 3068
ISSN (Print): 2151-2043
Original language: English
Links:
http://ma.ecsdl.org.proxy.findit.dtu.dk/content/MA2016-02/40/3068.abstract?sid=70825e1c-811f-45d9-8161-3689170919a2
Publication: Research - peer-review › Conference abstract in journal – Annual report year: 2016

Electrochemically Scavenging the Silica Impurities at the Ni-YSZ Triple Phase Boundary of Solid Oxide Cells
Silica impurity originated from the sealing or raw materials of the solid oxide cells (SOCs) accumulating at the Ni-YSZ triple phase boundaries (TPBs) is known as one major reason for electrode passivation. Here we report nanosilica precipitates inside Ni grains instead of blocking the TPBs when operating the SOCs at vertical $\bar{\text{v}} \geq 1.5 \text{ A cm}^{-2}$ for electrolysis of $\text{H}_2\text{O}/\text{CO}_2$. An electrochemical scavenging mechanism was proposed to explain this unique behavior: the removal of silica proceeded through the reduction of the silica to Si under strong cathodic polarization, followed by bulk diffusion of Si into Ni and reoxidation of Si in the Ni grain.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, University of Oslo, West Virginia University
Authors: Tao, Y. (Ekstern), Shao, J. (Intern), Cheng, S. (Ekstern)
Number of pages: 5
Pages: 17023-17027
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: A C S Applied Materials and Interfaces
Volume: 8
Issue number: 27
ISSN (Print): 1944-8244
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 8.15 SJR 2.784 SNIP 1.543
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 7.6 SJR 2.561 SNIP 1.536
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 2.262 SNIP 1.555 CiteScore 7.38
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.125 SNIP 1.636 CiteScore 6.88
Web of Science (2014): Indexed yes
Electrochemical Reduction of NO₂

General information
State: Published
Organisations: Fundamental Electrochemistry, Department of Energy Conversion and Storage, Shenzhen University
Authors: Shao, J. (Ekstern), Holtappels, P. (Intern), Kammer Hansen, K. (Intern)
Number of pages: 1
Publication date: 2016
Conference: The 229th ECS Meeting, San Diego, CA, United States, 29/05/2016 - 29/05/2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Electrochemical Society. Meeting Abstracts (Online)
Volume: MA2016-01
Article number: 1373
ISSN (Print): 2151-2043
Original language: English
Electronic versions:
Electrochemical_Reduction_of_NO2.pdf
Links:
http://ma.ecsdl.org/content/MA2016-01/28/1373.abstract?sid=abc96dbb-3b67-49ec-9588-ac0ca9a0cc45
Publication: Research - peer-review › Conference abstract in journal – Annual report year: 2016

Electrochemical removal of NOx using solid oxide cells

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Fundamental Electrochemistry
Authors: Kammer Hansen, K. (Intern), Traulsen, M. L. (Intern), Holtappels, P. (Intern)
Number of pages: 1
Publication date: 2016
Event: Abstract from Electrochemistry 2016, Goslar, Germany.
Main Research Area: Technical/natural sciences
Electronic versions:
Electrochemical removal
Publication: Research › Conference abstract for conference – Annual report year: 2016
Electrochemical Studies of Corrosion in Liquid Electrolytes for Energy Conversion Applications at Elevated Temperatures

Stainless steels (AISI 316, 321 and 347), high-nickel alloys (Hastelloy®C-276 and Inconel®625), tantalum, nickel, titanium, tungsten, molybdenum, niobium, platinum, and gold were tested for corrosion resistance in molten KH2PO4 (or KH2PO4-K2H2P2O7) as a promising electrolyte for the intermediate-temperature (200–400°C) water electrolysis. Pt, Ta, Nb, Ti, Inconel®625, and Ni demonstrated high corrosion resistance. Au and the rest of the tested materials were not corrosion resistant. It means that Ni, Ti and Inconel®625 may be used as relatively cheap construction materials for the intermediate-temperature water electrolyzer.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors
Authors: Nikiforov, A. V. (Intern), Petrushina, I. (Intern), Bjerrum, N. J. (Intern)
Pages: 89-100
Publication date: 2016

Host publication information
Title of host publication: High Temperature Corrosion
Publisher: InTechOpen
Editor: Ahmad, Z.
Chapter: 5
Main Research Area: Technical/natural sciences
Intermediate-temperature electrolysis, Bipolar plate, Nickel stability, Corrosion, Oxygen evolution, Molten salts
Electronic versions:
Electrochemical_Studies_of_Corrosion_in_Liquid.pdf
DOIs:
10.5772/64003

Bibliographical note
Published: September 7, 2016 under CC BY 3.0 license. © The Author(s).
Source: PublicationPreSubmission
Source-ID: 127149620
Publication: Research - peer-review › Book chapter – Annual report year: 2016

Electrodeposition of metallic 3D surface-profiles for superconductor tapes

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Imaging and Structural Analysis, Department of Physics
Authors: Wulff, A. C. (Intern), Jørgensen, P. S. (Intern), Nielsen, P. H. (Intern), Hansen, J. O. B. (Ekstern)
Number of pages: 1
Publication date: 2016
Main Research Area: Technical/natural sciences
Links:
http://www.sustain.dtu.dk/

Bibliographical note
Sustain Abstract M-16
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2016

Electronic Structure of Low-Dimensional Carbon $\Pi$-Systems

X-ray absorption spectroscopy (XAS) is combined with density functional theory (DFT) to determine the orbitals of one- and two-dimensional carbon $\Pi$-systems (lycopene, beta-carotene, retinal, retinol, retinoic acid, coronene, triphenylene). Considerable fine structure is observed for the transition from the C is level to the lowest unoccupied molecular orbital (LUMO) and explained by DFT. The wave functions of the one-dimensional chain molecules display the node structure of a vibrating string. The XAS transition energy is decomposed into contributions from the C is core level, the $\Pi^*$ final state, and the electron hole interaction. For the latter, we develop a simple model that accurately represents a full Delta-self-consistent field (ΔSCF) calculation. The distortion of the LUMO because of its interaction with the C is hole is investigated. These results illustrate the electronic states of prototypical $\Pi$-bonded carbon structures with low-dimensional character, such as those used in molecular complexes for solar cells, confined graphene structures, and molecular wires.
In this work we study the structural degradation of a laboratory Li-ion battery LiFePO4/C cathode by various electron microscopy techniques including low kV Focused Ion Beam (FIB)/Scanning Electron Microscopy (SEM) 3D tomography. Several changes are observed in FIB/SEM images of fresh and degraded cathodes, including cracks in the LFP particles, secondary disconnected particles, and agglomeration of CB. Low voltage (1 kV) SEM images show that the CB agglomerates have a different brightness than the fresh CB, due to charging effects. This suggests that the electronic conductivity of the CB agglomerates is low compared to that of the fresh CB particles. HRTEM analysis shows that fresh CB particles are quasi crystalline, whereas the LFP/CB interface in the degraded electrode shows amorphous carbon surrounding the LFP particles. The presence of the amorphous carbon is known to impede the electronic conductivity and thereby decreasing percolation in the cathode and reducing the electrode capacity.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry, Imaging and Structural Analysis, Atomic scale modelling and materials, Northwestern University
Number of pages: 11
Pages: 259-269
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Power Sources
Volume: 307
ISSN (Print): 0378-7753
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 7 SJR 2.202 SNIP 1.536
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 6.22 SJR 1.944 SNIP 1.5
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.9 SNIP 1.667 CiteScore 6.34
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.964 SNIP 2.042 CiteScore 6.3
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.975 SNIP 2.137 CiteScore 5.63
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Degradation mechanism, Focused ion beam scanning electron microscopy, Loss in electron percolation, Low accelerating voltage, Three-dimensional analysis of LiFePO4/Carbon electrode

Electron microscopy investigations.pdf

Electro-Oxidative Conversion and Process Intensification of Biomass derived 5-Hydroxymethylfurfural into 2,5-furandicarboxylic acid

Electro-Oxidative Conversion

General information
State: Published
Organisations: Fundamental Electrochemistry, Department of Energy Conversion and Storage
Authors: Joya, K. S. (Intern), Chatzichristodoulou, C. (Intern), Holtappels, P. (Intern)
Number of pages: 1
Publication date: 2016
Main Research Area: Technical/natural sciences
Electronic versions:

Electro-Oxidative Conversion

Publication: Research - peer-review › Journal article – Annual report year: 2016
Electroreduction of N2 to ammonia at ambient conditions on mononitrides of Zr, Nb, Cr, and V – A DFT guide for experiments

A rapid and facile reduction of nitrogen to achieve a sustainable and energy efficient production of ammonia is critical to its use as a hydrogen storage medium, chemical feedstock and especially for manufacturing inorganic fertilizers. For a decentralization of catalytic ammonia production, small-scale N2 reduction devices are required that are equipped with the most stable, selective and active catalysts that operate at low temperature and ambient pressure. Here, we report the development of new and cost-efficient catalysts, transition metal nitrides, which enable electrochemical reduction of molecular nitrogen to ammonia in aqueous media at ambient conditions with only a low applied bias. The most promising catalysts are VN, ZrN, NbN and CrN, which are identified among a range of transition metal nitride surfaces through a comprehensive density functional theory based analysis. All four nitrides are found to be more active towards nitrogen reduction than towards the competing hydrogen evolution reaction, in contrast to pure metal catalysts, which largely evolve hydrogen. Furthermore, their stability against poisoning and possible decomposition under operating conditions is also studied. Particular single-crystal surfaces are needed for ZrN, NbN and CrN because polycrystalline surfaces may result in decomposition of the whole catalyst. Polycrystalline surfaces of VN may, however, be used since the rocksalt (100) facet is predicted to produce ammonia via a Mars-van Krevelen mechanism with only a -0.5 V overpotential, thereby avoiding decomposition. We suggest that this is a promising step towards the development of a method for synthesizing ammonia cheaply, to prepare high-value-added nitrogenous compounds directly from air, water and electricity at ambient conditions. An additional benefit to the present analysis is that the method used in this work may be applicable to other aqueous phase catalytic reactions, where a Mars-van Krevelen mechanism is operative and product selectivity and activity are key catalytic criteria.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, University of Iceland, University of Otago
Authors: Abghoui, Y. (Ekstern), Garden, A. L. (Ekstern), Howalt, J. G. (Intern), Vegge, T. (Intern), Skúlason, E. (Ekstern)
Pages: 635–646
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: A C S Catalysis
Volume: 6
ISSN (Print): 2155-5435
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 11.49 SJR 4.921 SNIP 2.113
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 10.3 SJR 4.367 SNIP 2.081
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 3.973 SNIP 2.119 CiteScore 9.88
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 3.67 SNIP 2.02 CiteScore 8.74
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 3.301 SNIP 1.848 CiteScore 7.41
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Scopus rating (2012): SJR 2.729 SNIP 1.619 CiteScore 5.19
ISI indexed (2012): ISI indexed no
Web of Science (2012): Indexed yes
ISI indexed (2011): ISI indexed no
Original language: English
DOIs:
10.1021/acscatal.5b01918
Elucidating Batch-to-Batch Variation Caused by Homocoupled Side Products in Solution-Processable Organic Solar Cells

Conjugated polymers and small molecules based on alternating electron-donating (D) and electron-accepting (A) building blocks have led to state-of-the-art organic solar cell materials governing efficiencies beyond 10%. Unfortunately, the connection of D and A building blocks via cross-coupling reactions does not always proceed as planned, which can result in the generation of side products containing D-D or A-A homocoupling motifs. Previous studies have reported a reduced performance in polymer and small molecule solar cells when such defect structures are present. A general consensus on the impact of homocouplings on device performance is, however, still lacking as is a profound understanding of the underlying causes of the device deterioration. For differentiating the combined effect of molecular weight and homocouplings in polymer solar cells, a systematic study on a small molecule system (DTS(FBBTh2)2) is presented. The impact of homocouplings on nanomorphology, thermal, and electro-optical properties is investigated. It is demonstrated that small quantities of homocouplings (}
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 3.279 SNIP 1.837
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.898 SNIP 1.761
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 2.892 SNIP 1.836
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 3.11 SNIP 1.845
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 3.198 SNIP 1.946
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 2.787 SNIP 1.946
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 2.526 SNIP 1.996
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 2.688 SNIP 1.924
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 2.514 SNIP 1.873
Scopus rating (2001): SJR 2.354 SNIP 1.87
Scopus rating (2000): SJR 1.997 SNIP 1.635
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 2.148 SNIP 1.736

Original language: English
Chemical reactions, Conjugated polymers, Defects, Electronic properties, Molecules, Nanostructured materials, Optical properties, Organic polymers, Organic solar cells, Polymer solar cells, Batch-to-batch variations, Cross coupling reactions, Device performance, Electrooptical properties, Photoactive layers, Small molecule systems, Solar cell materials, Solution processable, Solar cells
DOIs:
10.1021/acs.chemmater.6b04143
Source: FindIt
Source-ID: 2349415299
Publication: Research - peer-review › Journal article – Annual report year: 2017

Emergent Material Science and Functionalities at Atomically-Engineered Oxide Interfaces

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Authors: Chen, Y. (Intern)
Number of pages: 177
Publication date: 2016

Publication information
Publisher: Department of Energy Conversion and Storage, Technical University of Denmark
ISBN (Print): 978-87-92986-45-0
Original language: English
Main Research Area: Technical/natural sciences

Bibliographical note
File available via Findit - DTU print collection
Source: PublicationPreSubmission
Source-ID: 125699957
Publication: Research › Doctoral thesis – Annual report year: 2016
Enhanced proton conductivity of niobium phosphates by interfacing crystal grains with an amorphous functional phase

Niobium phosphate is an interesting proton conductor operational in the intermediate temperature range. In the present work two forms of phosphates were prepared: an amorphous one with high specific area and a crystalline one with low specific surface area. Both phosphates exhibited very low proton conductivities. An activation process was developed to convert the phosphates into crystal grains with a phosphorus rich amorphous phase along the grain boundaries. As a result, the obtained niobium phosphates showed considerably enhanced and stable proton conductivities. The activation effect was prominent when the high surface area amorphous phosphate was used as the precursor. At 250 °C thus obtained niobium phosphate showed a high and stable conductivity of 0.03 S cm⁻¹ under dry atmosphere and of 0.06 S cm⁻¹ at a water partial pressure of 0.12 atm.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors, China University of Geosciences, Wuhan
Authors: Huang, Y. (Ekstern), Yu, L. (Ekstern), Li, H. (Ekstern), Wang, C. (Ekstern), Li, Q. (Intern), Shuai, Q. (Ekstern)
Number of pages: 5
Pages: 54-58
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Solid State Ionics
Volume: 294
ISSN (Print): 0167-2738
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 2.64 SJR 0.856 SNIP 0.952
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.41 SJR 0.75 SNIP 0.909
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.802 SNIP 1.016 CiteScore 2.5
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.837 SNIP 1.282 CiteScore 2.62
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.903 SNIP 1.269 CiteScore 2.35
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.051 SNIP 1.253 CiteScore 2.31
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.376 SNIP 1.615 CiteScore 2.96
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.46 SNIP 1.498
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.508 SNIP 1.483
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Epoxy-bonded La(Fe,Mn,Si)$_{13}$H$_{3}$ As A Multi Layered Active Magnetic Regenerator

The high magnetocaloric effect and tunability of the Curie temperature over a broad range makes La(Fe,Mn,Si)$_{13}$H$_{3}$ a promising magnetocaloric material for applications. Due to a volume change across the transition and the brittleness of the material as well as erosion due to fluid flow, the particles of the material may break apart during operation. In this context, we studied epoxy-bonded La(Fe,Mn,Si)$_{13}$H$_{3}$ regenerators, in a small versatile active magnetic regeneration (AMR) test device with a 1.1 T permanent magnet source. The magnetocaloric material was in the form of packed irregular particles (250-500 µm), which were mechanically held in place by an epoxy matrix connecting the particles, improving the mechanical integrity, while allowing a continuous porosity for the fluid flow. Water with 2 wt% ENTEK FNE as anti-corrosion additive was used as the heat transfer fluid for the epoxy-bonded regenerators. A series of AMRs was evaluated by varying the epoxy content in the range 1-4 wt%.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Vacuumschmelze GmbH & Co. KG
Authors: Neves Bez, H. (Intern), Navickaitė, K. (Intern), Lei, T. (Intern), Engelbrecht, K. (Intern), Barcza, A. (Ekstern), Bahl, C. (Intern)
Number of pages: 6
Publication date: 2016

Host publication information
Title of host publication: Proceedings of the 7th International Conference on Magnetic Refrigeration at Room Temperature
Publisher: International Institute of Refrigeration
Main Research Area: Technical/natural sciences
Magnetocaloric, Refrigeration, Epoxy-bonded, Layered regenerator, AMR
DOIs: 10.18462/iir.thermag.2016.0147
Publication: Research - peer-review › Article in proceedings – Annual report year: 2016

Evidence for lattice-polarization-enhanced field effects at the SrTiO$_3$-based heterointerface

Electrostatic gating provides a powerful approach to tune the conductivity of the two-dimensional electron liquid between two insulating oxides. For the LaAlO$_3$/SrTiO$_3$ (LAO/STO) interface, such gating effect could be further enhanced by a strong lattice polarization of STO caused by simultaneous application of gate field and illumination light. Herein, by
monitoring the discharging process upon removing the gate field, we give firm evidence for the occurrence of this lattice polarization at the amorphous-LaAlO$_3$/SrTiO$_3$ interface. Moreover, we find that the lattice polarization is accompanied with a large expansion of the out-of-plane lattice of STO. Photo excitation affects the polarization process by accelerating the field-induced lattice expansion. The present work demonstrates the great potential of combined stimuli in exploring emergent phenomenon at complex oxide interfaces.

**General information**
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Chinese Academy of Sciences
Authors: Li, Y. (Ekstern), R. Zhang, H. (Ekstern), Lei, Y. (Ekstern), Chen, Y. (Intern), Pryds, N. (Intern), Shen, B. (Ekstern), Sun, J. (Ekstern)
Number of pages: 6
Publication date: 2016
Main Research Area: Technical/natural sciences

**Publication information**
Journal: Scientific Reports
Volume: 6
Article number: 22418
ISSN (Print): 2045-2322
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 4.36 SJR 1.533 SNIP 1.245
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.63 SJR 1.692 SNIP 1.354
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 2.034 SNIP 1.597 CiteScore 5.3
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.163 SNIP 1.554 CiteScore 4.75
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.998 SNIP 1.57 CiteScore 4.06
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.531 SNIP 0.962 CiteScore 2.44
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
ISI indexed (2011): ISI indexed no
Original language: English
Electronic versions:
srep22418Evidence_for_lattice_polarization_enhanced_field_effects_at_the_SrTiO3_based_heterointerface.pdf
DOIs:
10.1038/srep22418

**Bibliographical note**
This work is licensed under a Creative Commons Attribution 4.0 International License. The images or other third party material in this article are included in the article’s Creative Commons license, unless indicated otherwise in the credit line; if the material is not included under the Creative Commons license, users will need to obtain permission from the license holder to reproduce the material. To view a copy of this license, visit http://creativecommons.org/licenses/by/4.0/
Publication: Research - peer-review › Journal article – Annual report year: 2016

**Evidence of weak superconductivity at the room-temperature grown LaAlO$_3$/SrTiO$_3$ interface**
The two-dimensional electron gas at the crystalline LaAlO$_3$/SrTiO$_3$ (c-LAO/STO) interface has sparked large interest due to its exotic properties, including an intriguing gate-tunable superconducting phase. While there is growing evidence of pronounced spatial inhomogeneity in the conductivity at STO-based interfaces, the consequences for superconductivity
remain largely unknown. We study interfaces based on amorphous LAO top layers grown at room temperature (a-LAO/STO) and demonstrate a superconducting phase similar to c-LAO/STO, however, with a gate-tunable critical temperature of 460 mK. The dependence of the superconducting critical current on temperature, magnetic field, and back-gate-controlled doping is found to be consistently described by a model of a random array of Josephson-coupled superconducting domains.

General information
State: Published
Organisations: Electrofunctional materials, Department of Energy Conversion and Storage, University of Copenhagen
Number of pages: 5
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Physical Review B
Volume: 93
Issue number: 18
Article number: 184504
ISSN (Print): 2469-9950
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 3.34 SJR 1.604 SNIP 1.04
Web of Science (2017): Indexed yes
Scopus rating (2016): CiteScore 3.16 SJR 2.339 SNIP 1.151
Web of Science (2016): Indexed yes
Scopus rating (2015): SJR 2.377 SNIP 1.13 CiteScore 2.8
Web of Science (2015): Indexed yes
Scopus rating (2014): SJR 2.762 SNIP 1.316 CiteScore 3.3
Web of Science (2014): Indexed yes
Scopus rating (2013): SJR 2.813 SNIP 1.326 CiteScore 3.55
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Scopus rating (2012): SJR 3.173 SNIP 1.378 CiteScore 3.57
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
Scopus rating (2011): SJR 3.326 SNIP 1.423 CiteScore 3.61
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
Scopus rating (2010): SJR 3.318 SNIP 1.447
Web of Science (2010): Indexed yes
Web of Science (2009): Indexed yes
Scopus rating (2008): SJR 2.923 SNIP 1.516
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 2.892 SNIP 1.588
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 2.62 SNIP 1.468
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 2.126 SNIP 1.156
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 2.012 SNIP 1.103
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 2.184 SNIP 1.179
Evolution of the electrochemical interface in high-temperature fuel cells and electrolysers

The critical region determining the performance and lifetime of solid oxide electrochemical systems is normally at the electrode side of the electrode/electrolyte interface. Typically this electrochemically active region only extends a few micrometres and for best performance involves intricate structures and nanocomposites. Much of the most exciting recent research involves understanding processes occurring at this interface and in developing new means of controlling the structure at this interface on the nanoscale. Here we consider in detail the diverse range of materials architectures that may be involved, describe the evolution of these interface structures and finally explore the new chemistries that allow control and manipulation of these architectures to optimize both performance and durability.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Fundamental Electrochemistry, Applied Electrochemistry, University of St Andrews
Number of pages: 13
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Nature Energy
Volume: 1
ISSN (Print): 2058-7546
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 7.025 SJR 17.765 CiteScore 25.21
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Web of Science (2016): Indexed yes
Original language: English
Electronic versions:
Irvine_et_al._2016_Evolution_of_the_electrochemical_interface_in_high_temperature_fuel_cells_and_electrolysers.pdf

Embargo ended: 12/07/2016
DOIs:
10.1038/NENERGY.2015.14
Source: PublicationPreSubmission
Source-ID: 119668671
Publication: Research - peer-review › Journal article – Annual report year: 2016

Exceptional durability enhancement of PA/PBI based polymer electrolyte membrane fuel cells for high temperature operation at 200°C
The incorporation of phosphotungstic acid functionalized mesoporous silica in phosphoric acid doped polybenzimidazole (PA/PBI) substantially enhances the durability of PA/PBI based polymer electrolyte membrane fuel cells for high temperature operation at 200°C.

**General information**
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors, Curtin University of Technology (Curtin University), Deakin University, University of Queensland
Number of pages: 6
Pages: 4019-4024
Publication date: 2016
Main Research Area: Technical/natural sciences

**Publication information**
Journal: Journal of Materials Chemistry A
Volume: 4
Issue number: 11
ISSN (Print): 2050-7488
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 9.61 SJR 3.488 SNIP 1.55
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 8.46 SJR 3.075 SNIP 1.479
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 2.62 SNIP 1.643 CiteScore 8.36
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.331 SNIP 1.514 CiteScore 7.27
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
ISI indexed (2013): ISI indexed no
Web of Science (2013): Indexed yes
Original language: English
Electronic versions:
Post_print_Exceptional_durability_enhancement_of_PA_PBI_based_polymer_electrolyte_membrane_fuel_cells_for_high_temperature_operation_at_200C.pdf
DOIs:
10.1039/c6ta01562j
Source: FindIt
Source-ID: 2292429884
Publication: Research - peer-review › Journal article – Annual report year: 2016

**Experimental and theoretical investigation of Cr_{1-x}Sc_xN solid solutions for thermoelectrics**
The ScN- and CrN-based transition-metal nitrides have recently emerged as a novel and unexpected class of materials for thermoelectrics. These materials constitute well-defined model systems for investigating mixing thermodynamics, phase stability, and band structure aiming for property tailoring. Here, we demonstrate an approach to tailor their thermoelectric properties by solid solutions. The trends in mixing thermodynamics and densities-of-states (DOS) of rocksalt-Cr1-xScxN solid solutions (0≤x≤1) are investigated by first-principles calculations, and Cr1-xScxN thin films are synthesized by magnetron sputtering. Pure CrN exhibits a high power factor, 1.7 ×10−3 Wm−1K−2 at 720K, enabled by a high electron concentration thermally activated from N vacancies. Disordered rocksalt-Cr1-xScxN solid solutions are thermodynamically stable, and calculated DOS suggest the possibility for power-factor improvement by Sc3d orbital delocalization on Cr3d electrons giving decreasing electrical resistivity, while localized Cr3d orbitals with a large DOS slope may yield an improved Seebeck coefficient. Sc-rich solid solutions show a large improvement in power factor compared to pure ScN, and all films have power factors above that expected from the rule-of-mixture. These results corroborate the theoretical predictions and enable tailoring and understanding of structure-transport-property correlations of Cr1-xScxN.
Experimental performance evaluation of sintered Gd spheres packed beds

Research in magnetic refrigeration heavily relies on the use of packed spheres in regenerators, however little investigation to verify that such non-monolithic arrangements guarantee a sufficiently constrained structure has yet been performed. This work presents a preliminary comparison of the performance of AMRs consisting of Gd spheres with diameters ranging from 450-550 microns partially sintered by Spark Plasma Sintering (SPS) to similar spheres, sorted in the same size range and from the same batch, but merely packed. Pressure drop is compared at uniform temperature and at a range of heat rejection temperatures and temperature spans. Performance is compared in terms of temperature span at a range of heat rejection temperatures (295-308 K) and 0 and 10 W cooling loads. Results show a moderate increase of pressure drop with the sintered spheres, while temperature spans were consistently 2.5-5 K smaller. These results are coherent with previously presented results [1].
Exploring product development possibilities and alternative uses of PV solar cells in Ghana

General information
State: Published
Organisations: Department of Management Engineering, UNEP DTU Partnership, Department of Energy Conversion and Storage, Secretariat, IT, Ashesi University, Kwame Nkrumah University of Science and Technology
Authors: Adomdza, G. K. (Ekstern), McBagonluri, F. (Ekstern), Kemasour, F. (Ekstern), Nygaard, I. (Intern), Hansen, U. E. (Intern), Lauritzen, H. (Intern)
Publication date: 2016

Publication information
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
Final_report_05092016.pdf

Bibliographical note
104.GHANA.809-200
Source: PublicationPreSubmission
Source-ID: 126116516
Publication: Research › Report – Annual report year: 2016

Exploring the efficiency potential for an active magnetic regenerator
A novel rotary state of the art active magnetic regenerator refrigeration prototype was used in an experimental investigation with special focus on efficiency. Based on an applied cooling load, measured shaft power, and pumping power applied to the active magnetic regenerator, a maximum second-law efficiency of 18% was obtained at a cooling load of 81.5 W, resulting in a temperature span of 15.5 K and a coefficient of performance of 3.6. A loss analysis is given, based on measured pumping power and shaft power together with theoretically estimated regenerator pressure drop. It is shown that, especially for the pressure drop, significant improvements can be made to the machine. However, a large part of the losses may be attributed to regenerator irreversibilities. Considering these unchanged, an estimated upper limit to the second-law efficiency of 30% is given by eliminating parasitic losses and replacing the packed spheres with a theoretical parallel plate regenerator. Furthermore, significant potential efficiency improvements through optimized regenerator geometries are estimated and discussed.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Technical University of Denmark
Authors: Eriksen, D. (Intern), Engelbrecht, K. (Intern), Haffenden Bahl, C. R. (Ekstern), Bjørk, R. (Intern)
Number of pages: 7
Pages: 527-533
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Science and Technology for the Built Environment
Volume: 22
Issue number: 5
ISSN (Print): 2374-4731
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 1.05
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.01
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.514 SNIP 0.731
Web of Science (2014): Indexed yes
Fabrication of doped Titania (TiO2) nanofibers to serve as catalysts in NH3-Selective CatalyticReduction (SCR)

In a context of significant interest for energy and environment, nanostructured-based ceramic materials areconsidered ideal candidates for the development of cost and energy efficient innovative systems. Such anattention is essentially due to the unique properties originating from the confinement of either one or moredimensions into the nanoscale level. Among others the large surface-to-volume ratio is a feature that greatlyincreases the reactivity of the nanomaterials towards gaseous species when compared with the non-nanodimensional materials. With this regards, catalysis is one of those applications that unquestionable benefitsfrom this novel feature. In addition, when nanofibers (1D nanostructure) are used as catalysts, the furtheradvantage of a self-supported wide open and well-interconnected porous structure is achieved.Herein we demonstrate nanofibers as catalysts for the removal of the NOx in exhausts via the NH3 SelectiveCatalytic Reduction (SCR) method. By combining electrospinning and sol-gel chemistry, materials areprocessed as nanofibers with the catalytic components (e. g. V2O5-WO3) incorporated as dopants intothesupporting anatase phase (e.g TiO2). Remarkable high NOx conversion efficiencies are obtained andassociated with the unique features deriving from the Synergism among the doping approach, the nanoscaleconfinement, and the nano-fibrous texture. A novel
Fabrication of thin film CZTS solar cells with Pulsed Laser Deposition

This project was about making CZTS solar cells using PLD for the fabrication of the absorber layer, and using standard techniques for the rest of the device. The solar cell is a very complicated device and all the steps in the fabrication are very important. It doesn't matter if PLD brings the best absorber layer, if one has a poor device processing the outcome will be disastrous. The converse holds true exactly in the same way. Developing the device-fabrication takes time, trials and errors. Unless one has a special PLD equipment for large area deposition, PLD's sample-throughput is too low to provide enough "dummy samples" to develop device processing. If one wants to try out PLD for making solar cells with a standard PLD setup, my suggestion is to first develop device processing with an alternative technique, e.g. sputtering, and with an established material, i.e. CIGS, easier than CZTS to handle. Once device processing is under control, the small area of the samples made with PLD may be a not-too-dramatic problem. CZTS as absorber layer is a polycrystalline material with a complicated structure that tolerates deviation from exact stoichiometry. It is very difficult to characterize such kind of material since many parameters can modify the optical and electronic properties: grain boundaries, point defects, disorder and secondary phases are just a few. When the CZTS layer is integrated in the solar cell, interface physics can also become very significant to the final device efficiency. As consequence, one cannot always distinguish a "good" or "bad" CZTS only using conventional techniques (Raman, SEM, x-ray diffraction, photoluminescence..) on the absorber layer alone. The only meaningful information comes from the full solar cell operation, but at this stage everything is coupled together behind the Quantum Efficiency (QE) curve. What do I learn by reading this thesis? You will learn how to deposit a thin film CZTS absorber layer with Pulsed Laser Deposition with the desired composition. In addition, you will see how material transfer in PLD, which is generally believed to be stoichiometric, can be very much non-stoichiometric. How to do it? I suggest to do PLD on a single sintered target (2CuS:ZnS:SnS) . The films are deposited at room temperature and then annealed in a furnace with some sulfur powder aside. The annealing step is as important as the PLD step to the final device efficiency. What is your best solar cells? With our own in-house device fabrication we reached a 2.6% conversion efficiency. With the absorber layer produced with our PLD setup followed by a well established annealing + device processing we reached a PLD record efficiency of 5.2%. The world record efficiency for this material is around 9%, with sputtering. Did you manage to get good quality CZTS? We cannot evaluate the performance of our annealing step afterwards. Preliminary results do not seem too encouraging. The main obstacle to this approach may be that droplets do not have enough thermal energy to dissociate and merge in the absorber layer. Any further suggestions? Learn by doing. Results from other group are more-often-than-not system dependent. Select your references very carefully. If the paper doesn't come from a group that has ever reported making solar cells, there is almost no point in reading it (and they are the vast majority).

Vox auctoritatis:

"," the thickness of annealed films was 1.7μm for CZTSSe, and 0.9μm for CZTS (significant cracks will develop for a thicker CZTS layer).", from a footnote in IBM's [34], Dec. 2015. And I really wish they had written this before.

"," even rather detailed materials characterization was not able to resolve the particular chemical products that led to the large differences in device performance. The devices in this study varied from 0.3% to 7.9% efficient, but no strong differences were observed by Raman, SEM, or EDS mapping at the surfaces and back contacts. This means that the causes of the electrical differences are on a smaller scale than the resolution of these techniques and could be, for example, very finely distributed secondary phases, changes in grain boundaries, or of course, point defects.\", from a paper by J. Scragg dated 2013 [29]. Which basically says that if you do not make a solar cell, you do not understand much about this material.

"of course you can talk about XRD, at some point you've got to write something to finish your PhD, but people mostly care about optical and electronic properties of this material, and of course, the efficiency of the solar cell above all". Private discussion with S. Siebentritt.

"," you just need to have the right composition in your precursors and the annealing pretty much does the job". Private discussion with T. Teodorov, from IBM's lab.
"[...] reproducibility of the results is an issue. Reproducibility of our best solar cells is below 30%". Private discussion with S. Tajima, from Toyota's lab.

**General information**

State: Published
Organisations: Department of Photonics Engineering, Optical Microsensors and Micromaterials, Department of Energy Conversion and Storage, Electrofunctional materials, Diode Lasers and LED Systems
Authors: Cazzaniga, A. C. (Intern), Schou, J. (Intern), Pryds, N. (Intern), Petersen, P. M. (Intern)
Number of pages: 128
Publication date: 2016

**Publication information**

Publisher: Technical University of Denmark (DTU)
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
Andrea_thesis_PLD_chalcogenides.pdf

**Relations**

Projects:
Fabrication of thin film CZTS solar cells with Pulsed Laser Deposition
Publication: Research › Ph.D. thesis – Annual report year: 2017

**Finite Bias Calculations to Model Interface Dipoles in Electrochemical Cells at the Atomic Scale**

The structure of an electrochemical interface is not determined by any external electrostatic field, but rather by external chemical potentials. This paper demonstrates that the electric double layer should be understood fundamentally as an internal electric field set up by the atomic structure to satisfy the thermodynamic constraints imposed by the environment. This is captured by the generalized computational hydrogen electrode model, which enables us to make efficient first-principles calculations of atomic scale properties of the electrochemical interface.

**General information**

State: Published
Organisations: Department of Energy Conversion and Storage, Department of Physics, Center for Nanostructured Graphene, University of Copenhagen
Authors: Hansen, M. H. (Intern), Jin, C. (Intern), Thygesen, K. S. (Intern), Rossmeisl, J. (Ekstern)
Number of pages: 7
Pages: 13485-13491
Publication date: 2016
Main Research Area: Technical/natural sciences

**Publication information**

Journal: Journal of Physical Chemistry C
Volume: 120
Issue number: 25
ISSN (Print): 1932-7447
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 4.58 SJR 2.135 SNIP 1.147
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.48 SJR 1.964 SNIP 1.195
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.886 SNIP 1.26 CiteScore 4.68
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.032 SNIP 1.447 CiteScore 5.08
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Flexible ITO-free organic solar cells applying aqueous solution-processed V2O5 hole transport layer: An outdoor stability study

Solution processable semiconductor oxides have opened a new paradigm for the enhancement of the lifetime of thin film solar cells. Their fabrication by low-cost and environmentally friendly solution-processable methods makes them ideal barrier (hole and electron) transport layers. In this work, we fabricate flexible ITO-free organic solar cells (OPV) by printing methods applying an aqueous solution-processed V2O5 as the hole transport layer (HTL) and compared them to devices applying PEDOT:PSS. The transparent conducting electrode was PET/Ag/PEDOT/ZnO, and the OPV configuration was PET/Ag/PEDOT/ZnO/P3HT:PC60BM/HTL/Ag. Outdoor stability analyses carried out for more than 900 h revealed higher stability for devices fabricated with the aqueous solution-processed V2O5.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Functional organic materials, Universidade Federal do Ceara, Universidad Autonoma de Barcelona, Universidade Estadual do Centro Oeste
Number of pages: 7
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: A P L Materials
Silver nanowires (AgNWs) were prepared on a 5g scale using either the well-known batch synthesis following the polyol method or a new flow synthesis method. The AgNWs were employed as semitransparent electrode materials in organic photovoltaics and compared to traditional printed silver electrodes based on micron sized silver flakes using life cycle analysis and environmental impact analysis methods. The life cycle analysis of AgNWs confirms that they provide an avenue to low-impact semitransparent electrodes. We find that the benefit of AgNWs in terms of embodied energy is less pronounced than generally assumed but that the toxicological and environmental benefits are significant.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Functional organic materials
Authors: Espinosa Martinez, N. (Intern), Søndergaard, R. R. (Intern), Jørgensen, M. (Intern), Krebs, F. C. (Intern)
Number of pages: 8
Pages: 893–899
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: ChemSusChem (Print)
Volume: 9
Issue number: 8
ISSN (Print): 1864-5631
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 6.86 SJR 2.538 SNIP 1.235
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 6.7 SJR 2.505 SNIP 1.311
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 2.53 SNIP 1.424 CiteScore 7.33
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.864 SNIP 1.663 CiteScore 7.97
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 2.561 SNIP 1.46 CiteScore 6.79
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Scopus rating (2012): SJR 3.054 SNIP 1.553 CiteScore 6.72
ISI indexed (2012): ISI indexed yes
Flow synthesis - the answer to reproducible high-performance conjugated polymers on the scale that R2R processing demands

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Organic Energy Materials
Authors: Helgesen, M. (Intern)
Publication date: 2016

Publication information
Media of output: Video
Original language: English
Publisher: DTU Energy
Main Research Area: Technical/natural sciences
Links:
https://youtu.be/S1KSjEnRjgM

Bibliographical note
Invited talk
Publication: Research - peer-review › Sound/Visual production (digital) – Annual report year: 2016

Formation of copper tin sulfide films by pulsed laser deposition at 248 and 355 nm
The influence of the laser wavelength on the deposition of copper tin sulfide (CTS) and SnS-rich CTS with a 248-nm KrF excimer laser (pulse length τ = 20 ns) and a 355-nm frequency-tripled Nd:YAG laser (τ = 6 ns) was investigated. A comparative study of the two UV wavelengths shows that the CTS film growth rate per pulse was three to four times lower with the 248-nm laser than the 355-nm laser. SnS-rich CTS is more efficiently ablated than pure CTS. Films deposited at high fluence have submicron and micrometer size droplets, and the size and area density of the droplets do not vary significantly from 248 to 355 nm deposition. Irradiation at low fluence resulted in a non-stoichiometric material transfer with significant Cu deficiency in the as-deposited films. We discuss the transition from a non-stoichiometric material transfer at low fluence to a nearly stoichiometric ablation at high fluence based on a transition from a dominant evaporation regime to an ablation regime.

General information
State: Published
Organisations: Department of Photonics Engineering, Optical Microsensors and Micromaterials, Department of Micro- and Nanotechnology, Silicon Microtechnology, Department of Energy Conversion and Storage, Electrofunctional materials,
From a magnet to a heat pump

The magnetocaloric effect (MCE) is the thermal response of a magnetic material to an applied magnetic field. Magnetic cooling is a promising alternative to conventional vapor compression technology in near room temperature applications and has experienced significant developments over the last five years. Although further improvements are necessary before the technology can be commercialized. Researchers were mainly focused on the development of materials and optimization of a flow system in order to increase the efficiency of magnetic heat pumps. The project, presented in this paper, is devoted to the improvement of heat pump and cooling technologies through simple tests of prospective regenerator designs. A brief literature review and expected results are presented in the paper. It is mainly focused on MCE technologies and provides a brief introduction to the magnetic cooling as an alternative for conventional vapor compression technology.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Pages: 73-79
Publication date: 2016
Main Research Area: Technical/natural sciences

Fuel Cells and Electrolyzers. Recent Progress at DTU Energy and the Role in a Sustainable Society

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors
Authors: Jensen, J. O. (Intern), Hu, Y. (Intern), Aili, D. (Intern), Zhong, L. (Intern), Cleemann, L. N. (Intern), Li, Q. (Intern)
Number of pages: 1
Publication date: 2016
Main Research Area: Technical/natural sciences
Functional Independent Scaling Relation for ORR/OER Catalysts

A widely used adsorption energy scaling relation between OH* and OOH* intermediates in the oxygen reduction reaction (ORR) and oxygen evolution reaction (OER), has previously been determined using density functional theory and shown to dictate a minimum thermodynamic overpotential for both reactions. Here, we show that the oxygen-oxygen bond in the OOH* intermediate is, however, not well described with the previously used class of exchange-correlation functionals. By quantifying and correcting the systematic error, an improved description of gaseous peroxide species versus experimental data and a reduction in calculational uncertainty is obtained. For adsorbates, we find that the systematic error largely cancels the vdW interaction missing in the original determination of the scaling relation. An improved scaling relation, which is fully independent of the applied exchange-correlation functional, is obtained and found to differ by 0.1 eV from the original. This largely confirms that, although obtained with a method suffering from systematic errors, the previously obtained scaling relation is applicable for predictions of catalytic activity.
Generating the optimal magnetic field for magnetic refrigeration

In a magnetic refrigeration device the magnet is the single most expensive component, and therefore it is crucially important to ensure that an effective magnetic field as possible is generated using the least amount of permanent magnets. Here we present a method for calculating the optimal remanence distribution for any desired magnetic field. The method is based on the reciprocity theorem, which through the use of virtual magnets can be used to calculate the optimal remanence distribution. Furthermore, we present a method for segmenting a given magnet design that always results in the optimal segmentation, for any number of segments specified. These two methods are used to determine the optimal magnet design of a 12-piece, two-pole concentric cylindrical magnet for use in a continuously rotating magnetic refrigeration device.

Globally Optimal Segmentation of Permanent-Magnet Systems

Permanent-magnet systems are widely used for generation of magnetic fields with specific properties. The reciprocity theorem, an energy-equivalence principle in magnetostatics, can be employed to calculate the optimal remanent flux density of the permanent-magnet system, given any objective functional that is linear in the magnetic field. This approach,
however, yields a continuously varying remanent flux density, while in practical applications, magnetic assemblies are realized by combining uniformly magnetized segments. The problem of determining the optimal shape of each of these segments remains unsolved. We show that the problem of optimal segmentation of a two-dimensional permanent-magnet assembly with respect to a linear objective functional can be reduced to the problem of piecewise linear approximation of a plane curve by perimeter maximization. Once the problem has been cast into this form, the globally optimal solution can be easily computed employing dynamic programming.

**General information**
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Secretariat, IT
Authors: Insinga, A. R. (Intern), Bjørk, R. (Intern), Smith, A. (Intern), Bahl, C. (Intern)
Number of pages: 16
Publication date: 2016
Main Research Area: Technical/natural sciences

**Publication information**
Journal: Physical Review Applied
Volume: 5
Issue number: 6
Article number: 064014
ISSN (Print): 2331-7019
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 4.62 SJR 2.089 SNIP 1.406
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.83 SJR 2.449 SNIP 1.602
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SNIP 1.492 SJR 2.345 CiteScore 3.31
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
BFI (2013): BFI-level 1
Original language: English
Electronic versions:
DOIs:
10.1103/PhysRevApplied.5.064014
Source: FindIt
Source-ID: 2306167446
Publication: Research - peer-review › Journal article – Annual report year: 2016

**Graphene layer encapsulated metal nanoparticles as a new type of non-precious metal catalysts for oxygen reduction**
Cheap and efficient non-precious metal catalysts for oxygen reduction have been a focus of research in the field of low-temperature fuel cells. This review is devoted to a brief summary of the recent work on a new type of catalysts, i.e., the graphene layer encapsulated metal nanoparticles. The discussion is focused on the synthesis, structure, mechanism, performance, and further research.

**General information**
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors
Authors: Hu, Y. (Intern), Zhong, L. (Intern), Jensen, J. O. (Intern), Li, Q. (Intern)
Number of pages: 4
Pages: 382-385
Publication date: 2016
Main Research Area: Technical/natural sciences

**Publication information**
Journal: Asia-Pacific Journal of Chemical Engineering
Volume: 11
Graphite and PMMA as pore formers for thermoplastic extrusion of porous 3Y-TZP oxygen transport membrane supports

A gas permeable porous support is a crucial part of an asymmetric oxygen transport membrane (OTM). Here, we develop feedstocks for thermoplastic extrusion of tubular, porous 3Y-TZP (partially stabilized zirconia polycrystals, (Y_2O_3)_{0.03}(ZrO_2)_{0.97}) ceramics, using graphite and/or polymethyl methacrylate (PMMA) as pore formers. The influence of pore former content and type, 3Y-TZP particle size and support sintering temperature on the microstructure, porosity and gas permeability were studied. Using at least 40 vol% pore former, consisting of graphite and PMMA in the volume ratio 2:1, tubes with gas permeability exceeding the target of 10^{-14} m^2 are obtained. In the temperature range 1250–1400°C the support gas permeability is insensitive to the sintering temperature, and the feedstocks shrink more than 15% during sintering, making them ideal for co-sintering with functional OTM layers. This demonstrates the suitability of thermoplastic extrusion for fabrication of porous 3Y-TZP OTM supports, or for other technologies requiring porous ceramics.

General information
State: Published
Scopus rating (2002): SJR 1.101 SNIP 1.184
Scopus rating (2001): SJR 1.236 SNIP 1.593
Scopus rating (2000): SJR 0.829 SNIP 1.179
Scopus rating (1999): SJR 1.11 SNIP 1.182
Original language: English
Porosity, Gas permeability, Thermoplastic extrusion, Oxygen transport membranes, YSZ
Electronic versions:
graphite.pdf. Embargo ended: 12/10/2017
DOIs:
10.1016/j.jeurceramsoc.2016.10.001
Source: FindIt
Source-ID: 2347584198
Publication: Research - peer-review › Journal article – Annual report year: 2016

Graphitic Layer Encapsulated Iron Based Non-precious Catalysts for the Oxygen Reduction Reaction

Proton exchange membrane fuel cells (PEMFCs) are highly efficient energy conversion devices, which can be in combination with hydrogen fuel providing a clean energy technology to produce electricity. One crucial challenge for this technology is the large cathodic overpotential due to the sluggish oxygen reduction reaction (ORR) kinetics. Carbon supported platinum (Pt/C) is the state-of-the-art benchmarking catalyst for PEMFCs since it exhibits the highest activity. However, the high cost and low abundance of noble metals have limited large-scale commercialization of the technology. Current efforts are made to develop non-precious metal catalysts (NPMCs) as a replacement to the Pt/C electrocatalysts.

In this thesis, a new type of NPMCs is synthesized by means of a dry autoclave with volatile ferrocene and cyanamide as precursors. The catalysts are morphologically featured by porous microspheres consisting of uniform metallic nanoparticles encapsulated in graphitic layers. The thesis work is conducted aiming at three major objectives: further optimization of the pyrolysis to achieve improved performance of catalysts, investigation of the complex Fe-containing components, and exploration of the possible active sites.

By systematic investigation of pyrolytic parameters i.e. temperature and duration, the best performance is achieved at 700 °C and 75 minutes, exhibiting a high catalytic activity in acid media (0.1 M HClO4) with an onset potential of 0.85 V at 0.1 mA cm⁻² and a mass specific kinetic current of 7.84 A g⁻¹ at 0.7 V vs. RHE. A good stability with 25 mV potential losses after 10,000 cycles of potential scan between 0.6 and 1.0 V has also been demonstrated.

The featuring morphology of the catalysts, i.e. the porous microspheres consisting of the graphitic layer encapsulated metal-containing nanoparticles, is essentially maintained during the pyrolysis of varied durations and temperatures. The metal-containing nanoparticles showed changes in the iron phases and their contents, as characterized by ⁵⁷Fe Mössbauer spectroscopy. The iron containing components include reduced metals (α-Fe and γ-Fe), oxide (γ-Fe₂O₃), carbide (Fe₃C) as well as a minor paramagnetic component due to Fe³⁺ (high spin) and/or possibly Fe²⁺ (low spin), likely coordinated with nitrogen (FeNx/C) as well identified for the Fe/N/C type catalysts in the literatures.

Quantitative determination of these metal containing components by low temperature ⁵⁷Mössbauer spectra shows that the content of the reduced metal component is steadily increasing with the pyrolytic time and temperature while the content of iron oxide is nearly constant. The most interesting finding is that the Fe₃C content shows a peak in both the temperature-varying and the duration-varying series of samples. The possible FeNx/C coordination phase, however, varies to a very limited extent for the studied samples.

The catalytic activities and mechanisms for ORR are evaluated by rotating disk electrode (RDE) and rotating ring-disk electrode (RRDE) voltammetry. In terms of the mass specific kinetic current density and half-wave potential, a strong correlation of the catalytic activity is established with the Fe₃C content within the entire composition range from 1.1 wt% to 4.5 wt% as well as with the FeNx/C content in a narrow range from 0.5 wt% to 0.85 wt%. Other iron containing components, i.e. α-Fe, γ-Fe and Fe₂O₃, showed no association with the ORR activity. It is concluded that, for the present catalysts, the recognized encapsulated iron carbide is most likely contributing to the ORR catalysis, in addition to the well identified N-coordinated Fe species.

More evidences are found from the catalyst synthesized from nitrogen free precursors. This catalyst, consisting of only carbon encapsulated iron-based nanoparticles, shows some, though low, ORR activity, which is enhanced by the post heat treatment in an ammonia atmosphere, indicating the contribution of the nitrogen functionalities.

Two anions in the electrolyte are used to probe the iron containing active sites towards the ORR, cyanide (CN⁻) in alkaline and thiocyanate (SCN⁻) in acidic medium, which seem supporting the above conclusions. These findings provide new insights to the encapsulation structure of Fe based nanocatalysts and therefore options for further development of NPMCs.

General information
State: Published
Guanidinium nonaflate as a solid-state proton conductor

Protic organic ionic plastic crystals (POIPCs) are a type of novel solid-state proton conductors. In this work, guanidinium nonaflate ([Gdm-H][NfO]) is reported to be a model POIPC. Its structure-property relationship has been investigated comprehensively. Infrared analysis of [Gdm-H][NfO] and its deuterated analogue [Gdm-D][NfO] confirms the complete formation of the protic salts. The cations in as-prepared [Gdm-D][NfO] are estimated to consist of [C(ND2)2(NHD)]+ and [C(ND2)3]+ with a molar ratio of around 1:1. The deuteration also proves that each guanidinium cation has six displaceable protons. Thermogravimetric analysis demonstrates that [Gdm-H][NfO] exhibits superior thermal stability in both nitrogen and air atmospheres. Isothermogravimetric analysis reveals its negligible vapor pressure with an estimated high enthalpy of vaporization (120.9 kJ mol⁻¹). Differential scanning calorimetry measurements of [Gdm-H][NfO] show four evident endothermic peaks prior to its melting transition at 186.2 °C with a low entropy of melting (17.70 J K⁻¹ mol⁻¹). Shortly before the onset temperature of melting transition (186.2 °C), partial melting (partial liquefaction) was observed via polarized optical microscopy in the temperature region of 176-186 °C while the reason for partial melting of ionic plastic crystals is not clear yet. Variable-temperature powder X-ray diffraction tests confirm the related solid-solid phase transitions and demonstrate that [Gdm-H][NfO] exhibits short-range disorder and long-range positional order in the plastic crystalline phases. Dielectric spectroscopy measurements show that its ionic conductivity reaches $2.1 \times 10^{-3}$ S cm⁻¹ at 185 °C. The proton conduction in the plastic crystalline phases of [Gdm-H][NfO] is assumed to happen via the vehicle mechanism. In the molten state, the proton conduction follows a combination of the vehicle mechanism and the Grotthuss mechanism (structural diffusion). In summary, due to their exceptional physicochemical properties, POIPCs like [Gdm-H][NfO] are promising electrolyte materials for high temperature (100-200 °C) proton exchange membrane fuel cells. In addition, POIPC-based solid-state proton conductors are also expected to find applications in sensors and other electrochemical devices.
**High Current Printed Transistor**

**General information**

State: Published  
Organisations: Department of Energy Conversion and Storage, Organic Energy Materials  
Authors: Pastorelli, F. (Intern), Schmidt, T. M. (Intern), Hösel, M. (Intern), Søndergaard, R. R. (Intern), Jørgensen, M. (Intern), Krebs, F. C. (Intern)  
Number of pages: 1  
Pages: 28  
Publication date: 2016

**Host publication information**

Title of host publication: Book of Abstracts. General Assembly of the Marie Curie Alumni Association 2016  
Publisher: Marie Curie Alumni Association  
Main Research Area: Technical/natural sciences  
Conference: General Assembly of the Marie Curie Alumni Association, Venice, Italy, 04/03/2016 - 04/03/2016  
Electronic versions:  
High_Current_Printed_Transistor.pdf  
Source: PublicationPreSubmission  
Source-ID: 127807214  
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2016

**High Current Printed Transistor: Roll-to-Roll Manufacture and Thermal Behavior**

**General information**

State: Published  
Organisations: Department of Energy Conversion and Storage, Organic Energy Materials  
Authors: Pastorelli, F. (Intern), Schmidt, T. M. (Intern), Hösel, M. (Intern), Søndergaard, R. R. (Intern), Jørgensen, M. (Intern), Krebs, F. C. (Intern)  
Number of pages: 1  
Publication date: 2016  
Event: Abstract from EMRS Spring Meeting 2016, Lille, France.  
Main Research Area: Technical/natural sciences  
Electronic versions:  
High_Current_Printed_Transistor_emrs.pdf  
Source: PublicationPreSubmission  
Source-ID: 127807028  
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2016
High ionic conductivity in confined bismuth oxide-based heterostructures

Bismuth trioxide in the cubic fluorite phase ($\delta$-Bi$_2$O$_3$) exhibits the highest oxygen ionic conductivity. In this study, we were able to stabilize the pure $\delta$-Bi$_2$O$_3$ at low temperature with no addition of stabilizer but only by engineering the interface, using highly coherent heterostructures made of alternative layers of $\delta$-Bi$_2$O$_3$ and Yttria Stabilized Zirconia (YSZ), deposited by pulsed laser deposition. The resulting [δ-Bi$_2$O$_3$=YSZ] heterostructures are found to be stable over a wide temperature range (500-750 °C) and exhibits stable high ionic conductivity over a long time comparable to the value of the pure $\delta$-Bi$_2$O$_3$, which is approximately two orders of magnitude higher than the conductivity of YSZ bulk.
Highly Interactive Surfaces on Impregnated electrodes - an in operando Raman Spectroscopy Study

General information
State: Published
Organisations: Fundamental Electrochemistry, Department of Energy Conversion and Storage, Montana State University
Authors: Traulsen, M. L. (Intern), Walker, R. (Ekstern), Holtappels, P. (Intern)
Number of pages: 1
Publication date: 2016
Main Research Area: Technical/natural sciences
Electronic versions:
Highly Interactive Surfaces.pdf
Publication: Research › Conference abstract for conference – Annual report year: 2016

Highly selective NOx reduction for diesel engine exhaust via an electrochemical system
It is challenging to reduce the nitrogen oxides (NOx) in diesel engine exhaust due to the inhibiting effect of excess oxygen. In this study, a novel electrochemical deNOx system was developed, which eliminated the need for additional reducing materials or a sophisticated controlling system as used in current diesel after-treatment techniques. The electrochemical system consisted of an electrochemical cell modified with NOx adsorbents and a diesel oxidation catalyst placed upstream of the cell. The system offers highly selective NOx reduction and a strong resistance to oxygen interference with almost zero emission of secondary pollutants.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, West Virginia University
Authors: Shao, J. (Intern), Tao, Y. (Ekstern), Kammer Hansen, K. (Intern)
Number of pages: 5
Pages: 36-40
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Electrochemistry Communications
Volume: 72
ISSN (Print): 1388-2481
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 1.013 SJR 1.606 CiteScore 4.56
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.53 SJR 1.626 SNIP 1.086
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.628 SNIP 1.176 CiteScore 4.77
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.832 SNIP 1.342 CiteScore 5.16
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.808 SNIP 1.422 CiteScore 4.97
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 2.316 SNIP 1.554 CiteScore 4.98
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 2.137 SNIP 1.604 CiteScore 5.14
ISI indexed (2011): ISI indexed yes
High-performance membrane-electrode assembly with an optimal polytetrafluoroethylene content for high-temperature polymer electrolyte membrane fuel cells

Although high-temperature polymer electrolyte membrane fuel cells (HT-PEMFCs) have a high carbon monoxide tolerance and allow for efficient water management, their practical applications are limited due to their lower performance than conventional low-temperature PEMFCs. Herein, we present a high-performance membrane-electrode assembly (MEA) with an optimal polytetrafluoroethylene (PTFE) content for HT-PEMFCs. Low or excess PTFE content in the electrode leads to an inefficient electrolyte distribution or severe catalyst agglomeration, respectively, which hinder the formation of triple phase boundaries in the electrodes and result in low performance. MEAs with PTFE content of 20 wt% have an optimal pore structure for the efficient formation of electrolyte/catalyst interfaces and gas channels, which leads to high cell performance of approximately 0.5 A cm⁻² at 0.6 V.

General information

State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors, Yonsei University, Korea Advanced Institute of Science & Technology, Korea Institute of Science and Technology
Authors: Jeong, G. (Ekstern), Kim, M. (Ekstern), Han, J. (Intern), Kim, H. (Ekstern), Shul, Y. (Ekstern), Cho, E. (Ekstern)
Number of pages: 5
Pages: 142-146
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Power Sources
Volume: 323
ISSN (Print): 0378-7753
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 7 SJR 2.202 SNIP 1.536
Web of Science (2017): Indexed yes
High-performance microchanneled asymmetric Gd<sub>0.1</sub>Ce<sub>0.9</sub>O<sub>1.95-δ</sub>-La<sub>0.6</sub>Sr<sub>0.4</sub>FeO<sub>3-δ</sub>-based membranes for oxygen separation

A microchanneled asymmetric dual phase composite membrane of 70 vol % Gd<sub>0.1</sub>Ce<sub>0.9</sub>O<sub>1.95-δ</sub>-La<sub>0.6</sub>Sr<sub>0.4</sub>FeO<sub>3-δ</sub> (CGO-LSF) was fabricated by a "one step" phase-inversion tape casting. The sample consists of a
thin dense membrane (100 μm) and a porous substrate including "finger-like" microchannels. The oxygen permeation flux through the membrane with and without catalytic surface layers was investigated under a variety of oxygen partial pressure gradients. At 900 degrees C, the oxygen permeation flux of the bare membrane was 1.6 (STP) ml cm(-2) min(-1) for the air/He-case and 10.10 (STP) ml cm(-2) min(-1) for the air/CO-case. Oxygen, flux measurements as well as electrical conductivity relaxation show that the oxygen flux through the bare membrane without catalyst is limited by the oxygen surface exchange. The surface exchange can be enhanced by introduction of catalyst on the membrane surface. An increase of the 50 150 oxygen flux of-4.49 (STP) mL cm(-2) min(-1) at 900 degrees C was observed when catalyst is added for the air/He-case. Mass transfer polarization through the finger-like support was confirmed to be negligible, which benefits the overall performance. A stable flux of 7.00 (STP) ml cm(-2) min(-1) was observed between air/CO/CO2 over 200 h at 850 degrees C. Partial surface decomposition was observed on the permeate side exposed to CO, in line with predictions from thermodynamic calculations. In a mixture of CO, CO2, H-2, and H2O at similar oxygen activity the material will according to the calculation not decompose. The microchanneled asymmetric CGO-LSF membranes show high oxygen permeability and chemical stability under a range of technologically relevant oxygen potential gradients.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Imaging and Structural Analysis, Ceramic Engineering & Science, University of Science and Technology of China, Jilin University
Number of pages: 13
Pages: 4548-4560
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: A C S Applied Materials and Interfaces
Volume: 8
Issue number: 7
ISSN (Print): 1944-8244
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 8.15 SJR 2.784 SNIP 1.543
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 7.6 SJR 2.561 SNIP 1.536
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 2.262 SNIP 1.555 CiteScore 7.38
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.125 SNIP 1.636 CiteScore 6.88
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.992 SNIP 1.548 CiteScore 6.05
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.199 SNIP 1.327 CiteScore 4.94
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.046 SNIP 1.404 CiteScore 4.41
ISI indexed (2011): ISI indexed no
Web of Science (2011): Indexed yes
Scopus rating (2010): SJR 1.597 SNIP 0.944
Web of Science (2010): Indexed yes
High Performance Nano-Ceria Electrodes for Solid Oxide Cells

In solid oxide electrochemical cells, the conventional Ni-based fuel-electrodes provide high electrocatalytic activity but they are often a major source of long-term performance degradation due to carbon deposition, poisoning of reaction sites, Ni mobility, etc. Doped-ceria is a promising mixed ionic-electronic conducting oxide that could solve these issues if it can be integrated into an appropriate electrode structure. Two new approaches to obtain high-performance nanostructured doped-ceria electrodes are highlighted. The first is an infiltration-based architecture with $\text{Ce}_0.8\text{Pr}_0.2\text{O}_{2-\delta}$ forming the active surfaces on a porous backbone with embedded electronic current collector material, yielding one of the highest performances reported for an electrode that operates either on fuel or oxidant. The second is a nano-$\text{Ce}_0.9\text{Gd}_0.1\text{O}_{2-\delta}$ thin film prepared by spin-coating, which provides an unprecedented electrode polarization resistance of $\sim 0.01 \, \Omega \, \text{cm}^2$ at 650 °C in $\text{H}_2/\text{H}_2\text{O}$. These results demonstrate that nano-ceria has the ability to achieve higher performance than Ni-based electrodes and show that the main challenge is obtaining sufficient electronic current collection without adding too much inactive material.
High Pressure Synthesis of Non-precious Metal ORR Catalysts for Fuel Cells

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors
Authors: Li, Q. (Intern)
Number of pages: 1
Publication date: 2016
Main Research Area: Technical/natural sciences

Relations
Activities:
High Pressure Synthesis of Non-precious Metal ORR Catalysts for Fuel Cells

High Temperature Alkaline Electrolysis Cells with Metal Foam Based Gas Diffusion Electrodes

Alkaline electrolysis cells operating at 250°C and 40 bar are able to convert electrical energy into hydrogen at very high efficiencies and power densities. In the present work we demonstrate the application of a PTFE hydrophobic network and Ag nanowires as oxygen evolution electrocatalyst in the metal foam based gas diffusion electrodes. A novel cell production method, based on tape casting and hot pressing, was developed which allows to increase the cell size from lab scale (1 cm²) to areas of 25 cm² or larger. The thickness of the electrolyte matrix could be adjusted to only 200 μm, achieving a serial resistance and total area specific resistance of only 60 mΩ cm² and 150 mΩ cm², respectively, at 200°C and 20 bar, yielding a record high current density of 3.75 A cm⁻² at a cell voltage of 1.75 V. Encouraging long-term stability was obtained over 400 h of continuous electrolysis. This novel cell concept promises more than a 10-fold improvement in power density, compared to conventional alkaline electrolysis cells, and thereby equivalent reduction in stack size and cost.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Fundamental Electrochemistry
Authors: Chatzichristodoulou, C. (Intern), Allebrod, F. (Intern), Mogensen, M. B. (Intern)
Number of pages: 5
Pages: F3036-F3040
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of The Electrochemical Society
Volume: 163
Issue number: 11
ISSN (Print): 0013-4651
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 3.48 SJR 1.267 SNIP 1.009
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.97 SJR 1.222 SNIP 0.963
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.115 SNIP 1.066 CiteScore 3.17
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.213 SNIP 1.25 CiteScore 3.36
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.169 SNIP 1.309 CiteScore 2.92
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.329 SNIP 1.281 CiteScore 2.61
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.331 SNIP 1.335 CiteScore 2.74
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.418 SNIP 1.304
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.442 SNIP 1.27
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.595 SNIP 1.41
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.569 SNIP 1.322
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.608 SNIP 1.535
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.523 SNIP 1.481
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.712 SNIP 1.7
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.971 SNIP 1.677
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 2.036 SNIP 1.618
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 1.663 SNIP 1.729
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 1.632 SNIP 1.7
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 1.6 SNIP 1.846

Original language: English
Alkaline, Ceramic separator, Electrolysis, High pressure, High temperature, Hydrogen, Metal foams, Power density, Stability
Moving away from fossil fuels requires harvesting more and more intermittent renewable energy resources and establishing a sustainable system for the production of chemicals. This brings forward the need for efficient large scale energy storage technologies and technologies for the conversion of renewable electricity to chemicals.

Electrochemical reactors can play a crucial role in this endeavor, since they can efficiently and reversibly transform electricity to high-value chemicals, and thus serve as energy storage and recovery devices for balancing the grid, while offering a means for the sustainable production of chemicals.

A novel type of alkaline electrochemical cell that can operate at elevated temperature and pressure has been developed that relies on corrosion resistant high temperature diaphragms, based on mesoporous ceramic membranes where aqueous KOH is immobilized by capillary forces. Raising the operating temperature offers a means to boost performance, as both ionic transport and reaction kinetics are exponentially activated with temperature. Indeed, we have demonstrated alkaline electrolysis cells operating at 200-250 °C and 20-50 bar at very high efficiencies and power densities.

This work will provide an overview of our efforts to develop components of such high temperature alkaline electrochemical reactors for different applications. Low-cost large-scale production methods have been successfully employed for the production of ceramic diaphragms and full cells. The influence of composition and microstructure on the long-term chemical stability and mechanical durability of the mesoporous ceramic membranes has been explored. Instrumentation for electrochemical testing at elevated pressures (up to 99 bar) and temperatures (up to 300 °C) with in-line chemical analysis has been established enabling experiments with gaseous or liquids reactants/products at cell sizes of up to 25 cm². Efforts are currently directed towards the investigation of the intrinsic activity of mixed oxides for the oxygen evolution reaction at elevated temperatures and pressures, and of the intrinsic activity, selectivity and stability of supported metal catalysts towards the electrocatalytic conversion of biomass derivatives to high-value chemicals. Finally, the use of selected electrocatalysts for the production of high performance electrodes will be reported.

High temperature and pressure alkaline electrochemical reactor for conversion of power to chemicals

High temperature and pressure alkaline electrochemical reactor for conversion of power to chemicals

High temperature AC conductance mapping for correlation of electrical properties with micron-sized chemical and microstructural features

High temperature AC conductance mapping is a scanning probe technique for resolving local electrical properties in microscopic areas. It is especially suited for detecting poorly conducting phases and for ionically conducting materials such as those used in solid oxide electrochemical cells. Secondary silicate phases formed at the edge of lanthanum strontium manganite microelectrodes are used as an example for correlation of chemical, microstructural and electrical properties with a spatial resolution of 1–2 µm to demonstrate the technique. The measurements are performed in situ in a controlled atmosphere high temperature scanning probe microscope at 650°C in air.
High temperature in operando and in situ spectroscopy on electrified surfaces and interfaces
Electrochemical cells, such as fuel cells, electrolyzers and batteries are considered as important technologies for storing electricity from renewable sources and also provide an efficient way of converting chemical energy into electricity. The processes in the electrodes are strongly influenced by the surface electrocatalytic properties, especially if instead of (or in addition to) hydrogen more complex reactants such hydrocarbons in form of alcohols, methane or higher hydro carbons are used as reactants. High temperature, solid state electrochemical cells based on an oxide ion conducting electrolyte are particularly attractive since hydrocarbon fuels in principle can be directly converted into electricity and vice versa with high efficiency. However, several side effects such as coking and poisoning with impurities e.g. sulfur on the fuel electrode, but also indication of changes in surface chemistry of oxide electrodes without contaminants have demanded a better insight into the electrode surface reactions and chemistries. Spectroscopic techniques can be applied to these cells but are still experimentally challenging due to the high temperature operation conditions. DTU Energy has in the recent years invested in specific equipment that allows investigating the electronic, electrical and chemical structure of surfaces under polarization at high temperatures and controlled atmospheres, allowing investigation of electrochemical cells and interfaces under close to operation conditions. The contribution will present selected examples of Raman spectroscopy, Kelvin probe and scanning probe microscopy applied to solid oxide electrochemical cells.

General information
State: Published
Organisations: Fundamental Electrochemistry, Department of Energy Conversion and Storage, Imaging and Structural Analysis
Publication date: 2016
Event: Abstract from EERA Annual Conference 2016, Birmingham, United Kingdom.
Main Research Area: Technical/natural sciences
Publication: Research › Conference abstract for conference – Annual report year: 2016

High temperature polymer electrolyte membrane fuel cells: Approaches, status, and perspectives
This book is a comprehensive review of high-temperature polymer electrolyte membrane fuel cells (PEMFCs). PEMFCs are the preferred fuel cells for a variety of applications such as automobiles, cogeneration of heat and power units, emergency power and portable electronics. The first 5 chapters of the book describe rationalization and illustration of approaches to high temperature PEM systems. Chapters 6 - 13 are devoted to fabrication, optimization and characterization of phosphoric acid-doped polybenzimidazole membranes, the very first electrolyte system that has demonstrated the concept of and motivated extensive research activity in the field. The last 11 chapters summarize the state-of-the-art of technological development of high temperature-PEMFCs based on acid doped PBI membranes including catalysts, electrodes, MEAs, bipolar plates, modelling, stacking, diagnostics and applications.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors, Department of Chemistry, Danish Power Systems ApS
Number of pages: 545
Publication date: 2016
Publisher: Springer
Homogenization of steady-state creep of porous metals using three-dimensional microstructural reconstructions

The effective steady-state creep response of porous metals is studied by numerical homogenization and analytical modeling in this paper. The numerical homogenization is based on finite element models of three-dimensional microstructures directly reconstructed from tomographic images. The effects of model size, representativeness, and boundary conditions on the numerical results are investigated. Two analytical models for creep rate of porous bodies are derived by extending the Hashin-Shtrikman bound and the Ramakrishnan-Arunchalam model in linear elasticity to steady-state creep based on nonlinear homogenization. The numerical homogenization prediction and analytical models obtained in this work are compared against reported measurements and models. The relationship between creep rate and porosity computed by homogenization is found to be bounded by the Hodge-Dunand model and the Hashin-Shtrikman creep model, and closely matched by the Gibson-Ashby compression and the Ramakrishnan-Arunchalam creep models. [All rights reserved Elsevier].

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors
Authors: Kwok, K. (Intern), Boccaccini, D. (Intern), Persson, Å. H. (Intern), Frandsen, H. L. (Intern)
Number of pages: 9
Pages: 38-46
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: International Journal of Solids and Structures
Volume: 78-79
ISSN (Print): 0020-7683
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 2.66 SJR 1.295 SNIP 1.516
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.8 SJR 1.548 SNIP 1.771
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.456 SNIP 1.893 CiteScore 2.66
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.603 SNIP 2.012 CiteScore 2.72
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.57 SNIP 2.104 CiteScore 2.6
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.534 SNIP 2.226 CiteScore 2.33
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Hydrogen Sulfide Tolerance in High Temperature PEMFCs

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors
Authors: Vassiliev, A. (Intern), Cleemann, L. N. (Intern), Li, Q. (Intern), Jensen, J. O. (Intern)
Number of pages: 1
Publication date: 2016
Conference: PRIME 2016/230th ECS Meeting, Honolulu, United States, 02/10/2016 - 02/10/2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Electrochemical Society. Meeting Abstracts (Online)
Volume: MA2016-02
Article number: 2813
ISSN (Print): 2151-2043
Original language: English
Links:
http://ma.ecsdl.org/content/MA2016-02/38/2813.abstract?sid=e4995d61-7422-498c-895c-bfd20f388e13

Bibliographical note
In situ diagnostics of the crystal-growth process through neutron imaging: application to scintillators

Neutrons are known to be unique probes in situations where other types of radiation fail to penetrate samples and their surrounding structures. In this paper it is demonstrated how thermal and cold neutron radiography can provide time-resolved imaging of materials while they are being processed (e.g. while growing single crystals). The processing equipment, in this case furnaces, and the scintillator materials are opaque to conventional X-ray interrogation techniques. The distribution of the europium activator within a BaBrCl:Eu scintillator (0.1 and 0.5% nominal doping concentrations per mole) is studied in situ during the melting and solidification processes with a temporal resolution of 5-7 s. The strong tendency of the Eu dopant to segregate during the solidification process is observed in repeated cycles, with Eu forming clusters on multiple length scales (only for clusters larger than ~50 μm, as limited by the resolution of the present experiments). It is also demonstrated that the dopant concentration can be quantified even for very low concentration levels (~ 0.1%) in 10 mm thick samples. The interface between the solid and liquid phases can also be imaged, provided there is a sufficient change in concentration of one of the elements with a sufficient neutron attenuation cross section. Tomographic imaging of the BaBrCl:0.1% Eu sample reveals a strong correlation between crystal fractures and Eu-deficient clusters. The results of these experiments demonstrate the unique capabilities of neutron imaging for in situ diagnostics and the optimization of crystal-growth procedures.
In situ time-of-flight neutron imaging of NiO-YSZ anode support reduction under influence of stress

This article reports on in situ macroscopic scale imaging of NiO-YSZ (YSZ is yttria-stabilized zirconia) reduction under applied stress - a phase transition taking place in solid oxide electrochemical cells in a reducing atmosphere of a hydrogen/nitrogen mixture and at operation temperatures of up to 1073 K. This process is critical for the performance and lifetime of the cells. Energy-resolved neutron imaging was applied to observe the phase transition directly with time and spatial resolution. Two different approaches are presented for using this imaging technique for the investigation of chemical and physical processes requiring controlled atmosphere and elevated temperature. The first type of measurement is based on alternating stages of short-term partial chemical reaction and longer neutron image acquisition, and the second type is a real in situ neutron imaging experiment. Results of applying energy-resolved neutron imaging with both approaches to the NiO-YSZ reduction investigation indicate enhancement of the reduction rate due to applied stress, which is consistent with the results of the authors' previous research.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Imaging and Structural Analysis, Mixed Conductors, European Spallation Source ESS AB, Xnovo Technology ApS, Rutherford Appleton Laboratory, University of California at Berkeley
Authors: Makowska, M. G. (Intern), Strobl, M. (Ekstern), Lauridsen, E. M. (Ekstern), Kabra, S. (Ekstern), Kockelmann, W. (Ekstern), Tremsin, A. (Ekstern), Frandsen, H. L. (Intern), Kuhn, L. T. (Intern)
In situ transmission electron microscopy for magnetic nanostructures

Nanomagnetism is a subject of great interest because of both application and fundamental aspects in which understanding of the physical and electromagnetic structure of magnetic nanostructures is essential to explore the magnetic properties. Transmission electron microscopy (TEM) is a powerful tool that allows understanding of both physical structure and micromagnetic structure of the thin samples at nanoscale. Among TEM techniques, in situ TEM is the state-of-the-art approach for imaging such structures in dynamic experiments, reconstructing a real-time nanoscale picture of the properties-structure correlation. This paper aims at reviewing and discussing in situ TEM magnetic imaging studies, including Lorentz microscopy and electron holography in TEM, applied to the research of magnetic nanostructures.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Imaging and Structural Analysis, University of Manchester
Authors: Ngo, D. (Ekstern), Kuhn, L. T. (Intern)
Number of pages: 16
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Advances in Natural Sciences: Nanoscience and Nanotechnology
Volume: 7
Issue number: 4
Article number: 045001
ISSN (Print): 2043-6254
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 0.625 SJR 0.442 CiteScore 1.7
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.403 SNIP 0.823 CiteScore 1.35
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.402 SNIP 0.628 CiteScore 1.3
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.474 SNIP 0.771 CiteScore 1.42
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.354 SNIP 0.611 CiteScore 1
ISI indexed (2013): ISI indexed no
Scopus rating (2012): SJR 0.339 SNIP 0.372
ISI indexed (2012): ISI indexed no
Scopus rating (2011): SJR 0.296 SNIP 0.266
ISI indexed (2011): ISI indexed no
Original language: English
In situ X-ray powder diffraction studies of the synthesis of graphene oxide and formation of reduced graphene oxide

Graphene oxide (GO) and reduced graphene oxide (rGO) are important materials in a wide range of fields. The modified Hummers methods, for synthesizing GO, and subsequent thermal reduction to rGO, are often employed for production of rGO. However, the mechanism behinds these syntheses methods are still unclear. We present an in situ X-ray diffraction study of the synthesis of GO and thermal reduction of GO. The X-ray diffraction revealed that the Hummers method includes an intercalation state and finally formation of additional crystalline material. The formation of GO is observed during both the intercalation and the crystallization stage. During thermal reduction of GO three stages were observed: GO, a disordered stage, and the rGO stage. The appearance of these stages depends on the heating ramp. The aim of this study is to provide deeper insight into the chemical and physical processes during the syntheses.
In situ X-ray scattering of perovskite solar cell active layers roll-to-roll coated on flexible substrates

In an effort to understand recent results showing differences between the power conversion efficiencies of lead halide (CH$_3$NH$_3$PbI$_{3-x}$Cl$_x$) solar cells on glass versus flexible substrates, this study investigates the influence that substrate and processing methods have on morphological and crystallographic development. Using our in situ slot-die micro roll-to-roll coater setup, we measured small and wide angle X-ray scattering in grazing incidence while the material dried, enabling us to follow the crystallization from just after the deposition and up to 25 minutes later. The data showed differing crystallographic developments between the substrates, especially seen through the behaviour of a crystalline precursor which survived longer on the flexible substrates than on glass. Additionally, the common degradation product PbI$_2$ was absent on the thickest flexible substrate. This leads us to conjecture that the flexible substrates absorb part of the solvent, thereby delaying evaporation and changing the solvent environment around the perovskite. As a further test, we produced solar cells with the same substrates and confirmed that the ones made on flexible substrates performed worse than those made on glass, but that when including an ITO layer in the stack it seemed to act as a buffer, whereby the solar cell performance was improved.

General information

State: Published
Impact of Prosumer Buildings and their Clusters on the Energy System – project outline

General information
State: Published
Organisations: Department of Civil Engineering, Section for Building Energy, Department of Energy Conversion and Storage
Authors: Larma, M. (Intern), Heller, A. (Intern), Pedersen, A. S. (Intern)
Number of pages: 1
Publication date: 2016
Main Research Area: Technical/natural sciences
Links:
http://www.sustain.dtu.dk/

Bibliographical note
Sustain Abstract L-10
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2016

Implementation of Constrained DFT for Computing Charge Transfer Rates within the Projector Augmented Wave Method
Combining constrained density function theory (cDFT) with Marcus theory is an efficient and promising way to address charge transfer reactions. Here, we present a general and robust implementation of cDFT within the projector augmented wave (PAW) framework. PAW pseudopotentials offer a reliable frozen-core electron description across the whole periodic table, with good transferability, as well as facilitate the extraction of all-electron quantities. The present implementation is applicable to two different wave function representations, atomic-centered basis sets (LCAO) and the finite-difference (FD) approximation utilizing real-space grids. LCAO can be used for large systems, molecular dynamics, or quick initialization, while more accurate calculations are achieved with the FD basis. Furthermore, the calculations can be performed with flexible boundary conditions, ranging from isolated molecules to periodic systems in one-, two-, or three-dimensions. As such, this implementation is relevant for a wide variety of applications. We also present how to extract the electronic coupling element and reorganization energy from the resulting diabatic cDFT-PAW wave functions for the parametrization of Marcus theory. Here, the combined method is applied to important test cases where practical implementations of DFT fail due to the self-interaction error, such as the dissociation of the helium dimer cation, and it is compared to other established cDFT codes. Moreover, for charge localization in a diamine cation, where it was recently shown that the commonly used generalized gradient and hybrid functionals of DFT failed to produce the localized state, cDFT produces qualitatively and quantitatively accurate results when benchmarked against self-interaction corrected DFT and high-level CCSD(T) calculations at a fraction of the computational cost.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, Center for Atomic-scale Materials Design, Department of Physics, Aalto University
Authors: Melander, M. (Intern), Jónsson, E. Ö. (Ekstern), Mortensen, J. J. (Intern), Vegge, T. (Intern), García Lastra, J. M. (Intern)
Number of pages: 12
Pages: 5367-5378
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Chemical Theory and Computation
Volume: 12
Issue number: 11
ISSN (Print): 1549-9618
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 5.25 SJR 2.497 SNIP 1.476
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 5.37 SJR 2.711 SNIP 1.51
Improved electrodes and gas impurity investigations on alkaline electrolysers

Alkaline water electrolysis for hydrogen production is a well-established technique but some technological issues regarding the coupling of alkaline water electrolysis and Renewable Energy Sources (RES) remain to be improved.

General information

State: Published
Organisations: Department of Energy Conversion and Storage, Imaging and Structural Analysis, German Aerospace Center, Flemish Institute for Technological Research, Hydrogenics Europe NV

Number of pages: 1
Publication date: 2016
Event: Poster session presented at The 21st World Hydrogen Energy Conference (WHEC), Zaragoza, Spain.
Main Research Area: Technical/natural sciences

Improving the Operational Stability of PBDTTTz-4 Polymer Solar Cells Modules by Electrode Modification

PBDTTTz-4 is employed in the ambient manufacturing of fully Roll-to-Roll organic solar cell modules. Modules are manufactured using a novel silver nanowire electrode or a previously reported carbon electrode. The average PCE of
carbon modules (3.07%) and AgNW modules (1.46%) shows that PBDTTTz-4 is a good candidate for upscaling. Stability measurements following the ISOS standards are used to compare the lifetime of the different modules. In all tests but one, the carbon modules are less stable. The higher stability of AgNW is attributed to the removal of the PEDOT:PSS in the front electrode. Finally during indoor light tests, a new degradation phenomenon is observed where bubbles are formed inside the modules contrary to previous reports of bubble formation by thermal expansion of trapped gas inside the barrier.
Improving the performance of district heating systems by utilization of local heat boosters

District Heating (DH) plays an important role in the Danish energy green transition towards the future sustainable energy systems. The new, 4th generation district heating network, the so-called Low Temperature District Heating (LTDH), tends to lower the supply temperature of the heat down to 40-50°C with return temperatures of 20-30°C. This kind of heating system has many advantages and among all of them, it allows utilization of the heat coming from low exergy heat sources, as well as to decrease the grid heat losses. Electrical energy driven heat sources are also integrated into the future LTDH grid as they will have the strategic role of connecting the heating system with the electrical energy coming from the intermittent and fluctuating renewable energy sources such as wind and solar power. In this paper, a case study of district heating systems is presented and analysed. The goal was to evaluate the possibilities to lower the forward temperature of the heat supply in order to reduce the heat losses of the system. Booster heat pumps are introduced to increase the water temperature close to the final users. A Matlab model was developed to simulate the state of the case study DH network in terms of mass flow rates, temperatures, and heat losses. After the model simulation, a new configuration of district heating with the introduction of three booster heat pumps was proposed. The new system's operation is determined based on a non-linear optimization problem in which the objective function was set to minimize the system's heat losses. This goal was achieved by lowering the forward temperature to 40°C and relying on the installed heat pumps to boost the water temperature to the admissible value needed for the domestic hot water preparation. Depending on the season, the optimized configuration allows decreasing the network heat losses in the range of 38-54%, higher reductions being achieved during colder seasons.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Sapienza University of Rome
Authors: Falcone, A. (Ekstern), Dominkovic, D. F. (Intern), Pedersen, A. S. (Intern)
Number of pages: 21
Publication date: 2016
Main Research Area: Technical/natural sciences
DOIs: 10.6084/m9.figshare.4595515.v1
Source: PublicationPreSubmission
Source-ID: 131716569
Publication: Research - peer-review › Paper – Annual report year: 2017

Incineration of organic solar cells: Efficient end of life management by quantitative silver recovery

Recovery of silver from the electrodes of roll-to-roll processed organic solar cells after incineration has been performed quantitatively with nitric acid. This procedure is more than 10 times faster than previous reports and the amount of acid needed for the extraction is reduced by a factor of 100-150. LCA studies show that the resulting environmental impacts from silver extraction of incinerated ashes are more favourable on almost all standard factors compared to extraction from shredded organic solar cells. The so lessened environmental impacts by efficient recovery fully justify the use of Ag as an electrode in scaled production of organic solar cells.

General information
State: Published
Infiltration of SOFC Stacks: Evaluation of the Electrochemical Performance Enhancement and the Underlying Changes in the Microstructure
Experimental SOFC stacks with 10 SOFCs (LSM-YSZ/YSZ/Ni-YSZ) were infiltrated with CGO and Ni-CGO on the air and fuel side, respectively in an attempt to counter degradation and improve the output. The electrochemical performance of each cell was characterized (i) before infiltration, (ii) after infiltration on the cathode side, and (iii) after the infiltration of the anode side. A significant performance enhancement was observed after the infiltration with CGO on the cathode, while the infiltration of the anode side with Ni-CGO had no significant effect on the electrochemical performance. After testing the cells were characterized by SEM and TEM/EELS. A thin layer of CGO nanoparticles around the LSM-YSZ backbone structure was found after infiltration. On the anode side nano sized Ni particles were found embedded in a CGO layer formed around the Ni-YSZ structure. EELS analysis showed that the oxidation state of the Ce ions is identical on the air and the fuel side.

**General information**

State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Applied Electrochemistry, Imaging and Structural Analysis, Case Western Reserve University, Topsoe Fuel Cell
Number of pages: 9
Pages: 80-88
Publication date: 2016
Main Research Area: Technical/natural sciences

**Publication information**

Journal: Fuel Cells
Volume: 16
Issue number: 1
ISSN (Print): 1615-6846
Ratings:
- BFI (2018): BFI-level 1
- Web of Science (2018): Indexed yes
- BFI (2017): BFI-level 1
- Scopus rating (2017): CiteScore 1.88 SJR 0.559 SNIP 0.748
- Web of Science (2017): Indexed yes
- BFI (2016): BFI-level 1
- Scopus rating (2016): CiteScore 1.79 SJR 0.495 SNIP 0.603
- Web of Science (2016): Indexed yes
- BFI (2015): BFI-level 1
- Scopus rating (2015): SJR 0.685 SNIP 0.779 CiteScore 2.02
- Web of Science (2015): Indexed yes
- BFI (2014): BFI-level 1
- Scopus rating (2014): SJR 0.615 SNIP 0.792 CiteScore 2.05
- Web of Science (2014): Indexed yes
- BFI (2013): BFI-level 1
- Scopus rating (2013): SJR 0.835 SNIP 0.833 CiteScore 1.99
- ISI indexed (2013): ISI indexed yes
- Web of Science (2013): Indexed yes
- BFI (2012): BFI-level 1
- Scopus rating (2012): SJR 1.24 SNIP 0.993 CiteScore 2.76
- ISI indexed (2012): ISI indexed yes
- Web of Science (2012): Indexed yes
- BFI (2011): BFI-level 1
- Scopus rating (2011): SJR 1.639 SNIP 1.247 CiteScore 3.31
- ISI indexed (2011): ISI indexed yes
- Web of Science (2011): Indexed yes
- BFI (2010): BFI-level 1
- Scopus rating (2010): SJR 1.623 SNIP 1.236
- Web of Science (2010): Indexed yes
- BFI (2009): BFI-level 1
- Scopus rating (2009): SJR 1.36 SNIP 1.108
Influence of pore former on porosity and mechanical properties of Ce$_{0.9}$Gd$_{0.1}$O$_{1.95}$ electrolytes for flue gas purification

Single layered porous Ce$_{0.9}$Gd$_{0.1}$O$_{1.95}$ electrolytes were fabricated by tape casting using different types, shapes and sizes of pore formers and their respective strength and stiffness were compared. The sintered bodies were characterized by scanning electron microscopy, mercury porosimetry, impulse excitation technique (Young modulus) and flexural strength measurements, to investigate the role of the different pore formers on the properties of the compounds. The compared techniques used to evaluate porosity give consistent results. The ratio between open and total porosities, evaluated from mercury porosimetry, varies depending on the used pore formers. The stiffness and strength of the compounds show an exponential dependency to the total porosity. By considering the open porosity instead (functional porosity), we observe that samples with platelets shaped pore formers have higher in-plane strength than spherical pore formers. An optimum can be found in term of Weibull strength and strain of samples obtained with the various pore formers by considering the dependency on the functional open porosity instead of the total porosity.

© 2015 Elsevier Ltd and Techna Group S.r.l. All rights reserved.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Ceramic Engineering & Science, Fundamental Electrochemistry, University of Erlangen-Nuremberg
Authors: Charlas, B. (Intern), Schmidt, C. G. (Intern), Frandsen, H. L. (Intern), Andersen, K. B. (Intern), Boccaccini, D. (Intern), Kammer Hansen, K. (Intern), Roosen, A. (Ekstern), Kaiser, A. (Intern)
Pages: 4546–4555
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Ceramics International
Volume: 42
ISSN (Print): 0272-8842
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 2.85 SJR 0.784 SNIP 1.167
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.88 SJR 0.844 SNIP 1.376
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.823 SNIP 1.281 CiteScore 2.64
Web of Science (2015): Indexed yes
Solid Oxide Fuel Cells are subjected to significant stresses during production and operation. The various stress-generating conditions impose strength requirements on the cell components, and thus the mechanical properties of the critical load-bearing materials at relevant operational conditions need to be characterized to ensure reliable operation. In this study, the effect of reduction temperature on microstructural stability, high temperature strength and elastic modulus of Ni-YSZ anode supports were investigated. The statistical distribution of strength was determined from a large number of samples (∼30) at each condition to ensure high statistical validity. It is revealed that the microstructure and mechanical properties of the Ni-YSZ strongly depend on the reduction temperature. Further studies were conducted to investigate the temperature dependence of the strength and elastic modulus for both the unreduced and reduced Ni(O)-YSZ anode supports. With increasing temperature, the strength and elastic modulus of the reduced Ni-YSZ specimens drop almost linearly. In contrast, the strength and elastic modulus of the unreduced NiO-YSZ remain almost constant over the investigated temperature range. Compared to the NiO-YSZ, a significantly lower strength and elastic modulus of the reduced Ni-YSZ is observed; while reduction leads to a remarkable increase in failure strain of the anode support.
Infrared ellipsometry study of the confined electrons in a high-mobility γ-Al₂O₃/SrTiO₃ heterostructure

With infrared ellipsometry we studied the response of the confined electrons in γ-Al₂O₃/SrTiO₃ (GAO/STO) heterostructures in which they originate predominantly from oxygen vacancies. From the analysis of a so-called Berreman mode, that develops near the highest longitudinal optical phonon mode of SrTiO₃, we derive the sheet carrier density, Nₛ, the mobility, μ, and the depth profile of the carrier concentration. Notably, we find that Nₛ and the shape of the depth profile are similar as in LaAlO₃/SrTiO₃ (LAO/STO) heterostructures for which the itinerant carriers are believed to arise from a polar discontinuity. Despite an order of magnitude higher mobility in GAO/STO, as obtained from transport measurements, the derived mobility in the infrared range exhibits only a twofold increase. We interpret this finding in terms of the polaronic nature of the confined charge carriers in GAO/STO and LAO/STO which leads to a strong, frequency-dependent interaction with the STO phonons.

General information

State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, University of Fribourg, Masaryk University
Authors: Yazdi-Rizi, M. (Ekstern), Marsik, P. (Ekstern), Mallett, B. P. P. (Ekstern), Dubroka, A. (Ekstern), Christensen, D. V. (Intern), Chen, Y. (Intern), Pryds, N. (Intern), Bernhard, C. (Ekstern)
Number of pages: 6
Publication date: 2016
Main Research Area: Technical/natural sciences
The Li-O₂ battery technology holds the promise to deliver a battery with significantly increased specific energy compared to today’s Li-ion batteries. As a cathode support material, reduced graphene oxide has received increasing attention in the Li-O₂ battery community due to the possibility of increased discharge capacity, increased battery cyclability, and decreased charging overpotential. In this article, we investigate the effect of water on a thermally reduced graphene, oxide cathode in a Li-O₂ battery. Differential electrochemical mass spectrometry reveals a decreased electron count for batteries with 1000 ppm water added to the electrolyte in comparison to dry batteries, indicating additional parasitic electrochemical processes. A comparable capacity of the wet and dry batteries indicates that the reaction mechanism in the Li-O₂ battery also depends on the surface of the cathode and not only on addition of water to the electrolyte as demonstrated by the solution-based mechanism. In situ synchrotron X-ray diffraction experiment using a new design of a capillary-based Li-O₂ cell with a thermally reduced graphene oxide cathode shows formation of LiOH along...
with Li$_2$O$_2$.

**General information**

State: Published  
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, Uppsala University  
Authors: Storm, M. M. (Intern), Christensen, M. K. (Intern), Younesi, R. (Ekstern), Norby, P. (Intern)  
Number of pages: 7  
Pages: 21211-21217  
Publication date: 2016  
Main Research Area: Technical/natural sciences

**Publication information**

Journal: Journal of Physical Chemistry C  
Volume: 120  
Issue number: 38  
ISSN (Print): 1932-7447  
Ratings:  
BFI (2018): BFI-level 1  
Web of Science (2018): Indexed yes  
BFI (2017): BFI-level 1  
Scopus rating (2017): CiteScore 4.58 SJR 2.135 SNIP 1.147  
Web of Science (2017): Indexed yes  
BFI (2016): BFI-level 1  
Scopus rating (2016): CiteScore 4.48 SJR 1.964 SNIP 1.195  
Web of Science (2016): Indexed yes  
BFI (2015): BFI-level 1  
Scopus rating (2015): SJR 1.886 SNIP 1.26 CiteScore 4.68  
Web of Science (2015): Indexed yes  
BFI (2014): BFI-level 1  
Scopus rating (2014): SJR 2.032 SNIP 1.447 CiteScore 5.08  
Web of Science (2014): Indexed yes  
BFI (2013): BFI-level 1  
Scopus rating (2013): SJR 2.143 SNIP 1.445 CiteScore 5.14  
ISI indexed (2013): ISI indexed yes  
Web of Science (2013): Indexed yes  
BFI (2012): BFI-level 1  
Scopus rating (2012): SJR 2.529 SNIP 1.461 CiteScore 4.98  
ISI indexed (2012): ISI indexed yes  
Web of Science (2012): Indexed yes  
BFI (2011): BFI-level 1  
Scopus rating (2011): SJR 2.339 SNIP 1.465 CiteScore 4.92  
ISI indexed (2011): ISI indexed yes  
Web of Science (2011): Indexed yes  
BFI (2010): BFI-level 1  
Scopus rating (2010): SJR 2.462 SNIP 1.362  
Web of Science (2010): Indexed yes  
BFI (2009): BFI-level 1  
Scopus rating (2009): SJR 2.158 SNIP 1.427  
Web of Science (2009): Indexed yes  
BFI (2008): BFI-level 1  
Scopus rating (2008): SJR 1.883 SNIP 1.04  
Web of Science (2008): Indexed yes  
Web of Science (2007): Indexed yes  
Web of Science (2006): Indexed yes  
Web of Science (2005): Indexed yes  
Web of Science (2004): Indexed yes
in-Situ Formed Ce₀.⁸Gd₀.₂O₁.₉ Barrier Layer on Yttria Stabilized Zirconia Back-Bone for Infiltrated Oxygen Electrodes

Solid oxide cells (SOCs) would be economically more favorable with lower operating temperature. Currently the target temperature is between 550 °C and 750 °C. Such low operation temperatures would reduce thermally activated degradation phenomena and would allow the use of cheaper materials. However, reduction of the operating temperature increases the ohmic and electrode polarization losses of the cells.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Applied Electrochemistry
Authors: Ovtar, S. (Intern), Chen, M. (Intern), Hauch, A. (Intern), Kiebach, W. (Intern)
Publication date: 2016
Conference: PRiME 2016/230th ECS Meeting, Honolulu, United States, 02/10/2016 - 02/10/2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Electrochemical Society. Meeting Abstracts (Online)
Volume: MA2016-02
Article number: 3049
ISSN (Print): 2151-2043
Original language: English
Links:
http://ma.ecsdl.org/content/MA2016-02/40/3049.abstract?sid=6f708a4c-d284-47b4-bd1f-63681204a5fd
Publication: Research - peer-review › Conference abstract in journal – Annual report year: 2016

In-situ, long-term operational stability of organic photovoltaics for off-grid applications in Africa

This paper presents a field-trial of organic photovoltaic (OPV) technology used within a practical application for rural electrification in Rwanda. Fourteen, large area, flexible, ITO-free, roll-to-roll processed OPV modules, encapsulated with low-cost materials, were installed on corrugated steel roofs at two sites in a rural village in Southern Rwanda and subject to continuous monitoring. This field-trial exposed modules to very high levels of insolation, in particular in the UV, high temperatures and heavy rainfall. Results show that the modules exhibit practical lifetimes (to degrade by 20% of their initial capacity) of between 2 and 5 months, a value 5-6 times lower than control modules kept both in the dark and outdoors in Roskilde, Denmark. Degradation was primarily the result of extensive delamination caused by failure of the non-UV stable encapsulation, which led to decay in the FF, Voc and Isc of the module.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Functional organic materials, Imperial College London, MeshPower Limited
Number of pages: 10
Pages: 284-293
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Solar Energy Materials and Solar Cells
Volume: 149
ISSN (Print): 0927-0248
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
Failure mechanisms, Field testing, Off-grid application, Outdoor testing in Africa, Polymer solar cell modules

DOIs:
10.1016/j.solmat.2016.01.036

Bibliographical note
This work was supported by Climate-KIC and the European Commission's CHEETAH Project (FP7-Energy-2013- Grant no. 609788)
**In-situ SEM electrochemistry and radiolysis**

Electron microscopy is a ubiquitous technique to see effects which are too small to see with traditional optical microscopes. Recently it has become possible to also image liquid samples by encapsulating them from the vacuum of the microscope and a natural evolution from that has been to include microelectrodes on the windows to enable studies of electrochemical processes. In this way it is possible to perform in-situ electrochemical experiments such as electroplating and charge and discharge analysis of battery electrodes.

In a typical liquid cell, electrons are accelerated to sufficiently high energies to traverse a thin window made by a silicon nitride membrane, and interact with the sample immersed in liquid. In transmission electron microscopy (TEM) the majority of the electrons continue through the sample to form an image. In scanning electron microscopy (SEM) a fraction of the electrons are backscattered and an image is reconstructed by the microscope. But the high energy electrons are a form of ionising radiation which can significantly affect the chemistry in liquid experiments. Ionising radiation can split water, produce radicals, reduce dissolved metal ions to metal particles, and more. It is therefore essential to understand and control the radiolytic processes that results from in-situ electron microscopy experiments.

Although radiolysis has been studied extensively in connection with the advent of e.g. nuclear reactors the information obtained for that purpose often has to be extrapolated many orders of magnitude to reach the radiation conditions of the extremely focused beam of typical electron microscopes. To date there is a distinct lack of direct measurements and quantification of the radiolytic conditions for in-situ liquid cells.

In this thesis an electrochemical in-situ SEM cell is used to study the radiolytic effects of the electron beam. Potentiometric measurements in-situ demonstrate that the electrolyte contains hydrogen upon irradiation, and that the ratio of H$_2$O$_2$ to H$_2$ is only 1:2.5, much less than the predicted ratio of 1.1.1. Electrochemical impedance spectroscopy (EIS) measurements between two electrodes when irradiating at an average intensity of 6 MGy/s indicate that the conductivity may be at least 200 $\mu$S/cm, two orders of magnitude higher than what would be expected from H$^+$ alone. Finally, the radiolytic yield of copper is measured by gradually increasing the radiation intensity until copper precipitated. Based on the amount of backscattered electrons it has been possible to quantify the amount of reduced copper, resulting in an average radiolytic yield per 100 eV of deposited energy (g-value) of 0.05, lower than the value of 4.4 seen in pulse radiolysis experiments. During the course of these studies it has also been possible to improve on the EC-SEM system. This has resulted in pyrolysed carbon electrodes, which offer the benefit of stability at 0.75 V higher potentials than traditional gold thin-film electrodes.

With the quantitative insight into the radiolytic conditions in liquid electron microscopy cells that this thesis provides it may be possible to design and analyse experiments where such effects are correctly accounted for. The results are therefore of high value for the in-situ community who until now have had to rely on only limited experimental data in combination with theoretical predictions that have been extrapolated several orders of magnitude.

**General information**

*State: Published*
*Organisations: Department of Micro- and Nanotechnology, Molecular Windows, Department of Energy Conversion and Storage, Center for Electron Nanoscopy*
*Authors: Møller-Nilsen, R. E. R. (Intern), Mølhave, K. (Intern), Norby, P. (Intern), Wagner, J. B. (Intern)*
*Number of pages: 112*
*Publication date: 2016*

**Publication information**

*Publisher: DTU Nanotech*
*Original language: English*
*Main Research Area: Technical/natural sciences*
*Electronic versions: RolfMollerNilsen_PhD_thesis_1.pdf*

**Relations**

*Projects: In-situ SEM electrochemistry and radiolysis*
*Source: PublicationPreSubmission*
*Source-ID: 127629530*
*Publication: Research › Ph.D. thesis – Annual report year: 2016*
it possible to undertake analysis during exposure to the SOFC/SOEC sample of reactive gas flow, elevated temperatures and electrical biasing in combination. This allows the study of nanostructure development under temperature and electrode polarisation conditions similar to operation conditions. In this work, we have for the first time performed in-situ analysis of a symmetric cell inside a TEM under different configurations. In order to be able to perform in-situ experiments while drawing a current through the sample, we used a homemade TEM chip [5,6] and an 80-300kV Titan ETEM (FEI Company) equipped with an image corrector and a differential pumping system. A symmetric cell was prepared by depositing a cell consisting of three thin films on a strontium titanate (STO) single crystal substrate by pulsed laser deposition (PLD). Lanthanum strontium cobaltite La0.6Sr0.4CoO3-δ (LSC) was chosen as electrode and yttria stabilized zirconia ZrO2: 8% mol Y2O3 (YSZ) as electrolyte, see figure 1. High resolution TEM analysis on PLD samples after the deposition, did not reveal any second phase formation at the interface between YSZ and LSC. The in-situ experiment was firstly conducted in vacuum at temperature between 25 oC and 900 oC. Secondly, it was repeated in presence of oxygen with an oxygen partial pressure of about 2 mbar and a maximum temperature of 750 oC. Subsequently, the symmetric cell will be exposed to oxygen at 600 oC and 1 V overpotential within the ETEM. In order to do that, a symmetric cell has been placed on the chip with the use of a focus ion beam (FIB) microscope, see figure 2. To do so, a lamella was first extracted by the bulk sample and attached to a conventional TEM grid. Afterwards, the grid was tilted by 90 degrees and the lamella was detached once again and placed on the chip. STEM-EDS investigation was used for ex-situ post mortem analysis. Finally, a bulk symmetric cell, coming from the same batch as the in-situ treated TEM samples, was tested in a furnace with similar environmental conditions. This comparison is vital for distinguishing possible surface diffusion effects caused by having a thin lamella for in-situ TEM analysis. Electrochemical properties were also investigated by electrochemical impedance spectroscopy (EIS). In the figure 3 the cell was heat treated at 400 oC in vacuum, whereas in figure 4, the cell was treated at the same temperature but in presence of oxygen, with PO2 of 2 mbar. Comparing the two figures, the cell exposed to oxygen showed structural changes in the LSC thin film in comparison with the sample heated in vacuum. These changes refer to the formation of grains as is confirmed by electron diffraction patterns.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Imaging and Structural Analysis, Fundamental Electrochemistry, Department of Micro- and Nanotechnology, Molecular Windows, Electrofunctional materials, Center for Electron Nanoscopy
Authors: Gualandris, F. (Intern), Simonsen, S. B. (Intern), Mogensen, M. B. (Intern), Mølhave, K. (Intern), Sanna, S. (Intern), Wagner, J. B. (Intern), Kuhn, L. T. (Intern)
Number of pages: 2
Publication date: 2016
Event: Abstract from 16th European Microscopy Congress 2016, Lyon, France.
Main Research Area: Technical/natural sciences
Electronic versions:
Lione_Abstract_PDF.pdf

Relations
Activities:
IN-SITU TRANSMISSION ELECTRON MICROSCOPY ON OPERATING ELECTROCHEMICAL CELLS
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2017

In SITU Transmission Electron Microscopy on Operating Electrochemical CELLS
Solid oxide cells (SOC) have the potential of playing a significant role in the future efficient energy system scenario. In order to become widely commercially available, an improved performance and durability of the cells has to be achieved [1]. Conventional scanning and transmission SEM and TEM have been often used for ex-situ post mortem characterization of SOFCs and SOECs [2,3]. However, in order to get fundamental insight of the microstructural development of SOFC/SOEC during operation conditions in situ studies are necessary [4].

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Imaging and Structural Analysis, Fundamental Electrochemistry, Department of Micro- and Nanotechnology, Molecular Windows, Electrofunctional materials, Center for Electron Nanoscopy, Nagoya University
Authors: Gualandris, F. (Intern), Simonsen, S. B. (Intern), Mogensen, M. B. (Intern), Mølhave, K. (Intern), Sanna, S. (Intern), Wagner, J. B. (Intern), Muto, S. (Ekstern), Higuchi, K. (Ekstern), Kuhn, L. T. (Intern)
Publication date: 2016
Conference: PRIME 2016/230th ECS Meeting, Honolulu, United States, 02/10/2016 - 02/10/2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Electrochemical Society. Meeting Abstracts (Online)
Volume: MA2016-02
Article number: 2976
Interface-Induced Renormalization of Electrolyte Energy Levels in Magnesium Batteries

A promising strategy for increasing the energy density of Li-ion batteries is to substitute a multivalent (MV) metal for the commonly used lithiated carbon anode. Magnesium is a prime candidate for such a MV battery due to its high volumetric capacity, abundance, and limited tendency to form dendrites. One challenge that is slowing the implementation of Mg-based batteries, however, is the development of efficient and stable electrolytes. Computational screening for molecular species having sufficiently wide electrochemical windows is a starting point for the identification of optimal electrolytes. Nevertheless, this window can be altered via interfacial interactions with electrodes. These interactions are typically omitted in screening studies, yet they have the potential to generate large shifts to the HOMO and LUMO of the electrolyte components. The present study quantifies the stability of several common electrolyte solvents on model electrodes of relevance for Mg batteries. Many-body perturbation theory calculations based on the G0W0 method were used to predict shifts in a solvent's electronic levels arising from interfacial interactions. In molecules exhibiting large dipole moments, our calculations indicate that these interactions reduce the HOMO-LUMO gap by ∼25% (compared to isolated molecules). We conclude that electrode interactions can narrow an electrolyte's electrochemical window significantly, thereby accelerating redox decomposition reactions. Accounting for these interactions in screening studies presents an opportunity to refine predictions of electrolyte stability.
Intermediate Phase Study on YBCO Films Coated by Precursor Solutions With F/Ba Atomic Ratio of 2

In the chemical solution deposition process of YBCO superconducting films, fluorine is widely regarded to be of significant importance in avoiding the formation of BaCO₃, which hinders the growth of high-quality YBCO films. On the other hand, great efforts have been made to decrease the fluorine content in the precursor solution due to the environmental contaminations of the fluorinated gaseous by-products. In this study, we demonstrate that an F/Ba atomic ratio of 2 in the precursor solution is sufficient according to the results of energy dispersive spectrometry and attenuated Fourier transform infrared studies. The intermediate phase evolution prior to the end of the sintering stage is also investigated by X-ray diffractometry and scanning electron microscopy. Liquid-like structures are observed, which are proposed to be responsible for the film densification in the early stage of YBCO formation. The formation of YBCO is accompanied by the consumption of oxygen-doped BaF₂ (BOF), which is found to be highly textured. Moreover, in the early stage of YBCO formation, the crystallinity and texture of BOF enhance despite its consumption. After a full heat treatment, YBCO films with Jc of 5 MA/cm² (77 K, 0 T) could be routinely obtained on lanthanum aluminate single-crystal substrates.
Intermediate Temperature Proton Conductors – Why and How

The current technologies of fuel cells and electrolysers are based on ionic conducting electrolyte materials exclusively operational either in the low (20 - 200ºC) or high (600 - 1000ºC) temperature ranges. The intermediate temperature window, especially between 200 and 400 ºC, is still only represented by early fundamental material research for ionic electrolytes. Such materials, most likely based on proton conductors, are expected to bring a new generation of the technologies: fuel cells by direct oxidation or internal splitting of biofuels such as methanol and ethanol, as well as efficient water electrolyzer, preferably a CO2 co-electrolyzer for generation of organic liquid fuels. Such technologies are of essential simplicity and allow for kinetic enhancement so that the need for precious metal catalysts as in low temperature
systems might be eliminated. At the same time, this temperature range is low enough to have a wide selection of materials for cell and stack construction, and with potential long-term durability. This talk will briefly outline the recent work at DTU based on acid-base complexes and metal phosphates.

Introduction

The papers in this special issue focus on the topic of organic nanophotonics. Since early works in the 1980s, significant advances have been made in organic materials with semiconducting and photonic properties due to the development of materials/device technologies on the nanoscale. The most impressive outcomes include organic light-emitting devices (OLEDs) that are now competing with the well-established liquid crystal display technology in the mobile and television markets. In addition, organic solar cells (OSCs) offer the potential to create new paradigms for ultrathin and lightweight plastic solar modules in the coming flexible electronics era. Further developments are ongoing across a broad range of organic nanophotonics topics including organic laser devices, organic phototransistors, organic plasmonic devices, etc. This issue introduces recent cutting-edge research from the fast-breaking area of organic nanophotonics. The subject in this special issue includes organic lasers, OLEDs, organic photovoltaics, organic phototransistors, microcavities, and related materials. In particular, most papers included in this special issue offer insights into technology innovations including flexible optoelectronics. We trust that readers will benefit from the timely and in-depth research presented in this special issue and get an insight into future nanophotonics directions with organic and related materials.
Investigation of CeO₂ Buffer Layer Effects on the Voltage Response of YBCO Transition-Edge Bolometers

The effect on the thermal parameters of superconducting transition-edge bolometers produced on a single crystalline SrTiO₃ (STO) substrate with and without a CeO₂ buffer layer was investigated. Metal-organic deposition was used to deposit the 20-nm CeO₂ buffer layer, whereas RF magnetron sputtering was applied to fabricate 150-nm-thick superconducting YBa₂Cu₃O₇₋ₓ (YBCO) thin film. The critical transition temperature for both of the YBCO films was 90 K, and the transition width was ∼1.9 K. The bolometers fabricated from these samples were characterized with respect to the voltage phase and amplitude responses, and the results were compared with that of simulations conducted by applying a one-dimensional thermophysical model. It was observed that adding the buffer layer to the structure of the bolometer results in an increased response at higher modulation frequencies. Results from simulations made by fitting the thermal parameters in the model with and without an additional CeO₂ layer were found to be in agreement with the experimental observations.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Sharif University of Technology
Authors: Mohajeri, R. (Ekstern), Nazifi, R. (Ekstern), Wulff, A. C. (Intern), Vesaghi, M. A. (Ekstern), Grivel, J. (Intern), Fardmanesh, M. (Ekstern)
Number of pages: 4
Publication date: 2016
Main Research Area: Technical/natural sciences
Investigation of the bonding strength and bonding mechanisms of SOFCs interconnector-electrode interfaces

General information
State: Published
Organisations: Mixed Conductors, Department of Energy Conversion and Storage, Applied Electrochemistry, Brno University of Technology, Academy of Sciences of the Czech Republic, Università degli Studi di Modena e Reggio Emilia
Authors: Boccaccini, D. N. (Intern), Sevecek, O. (Ekstern), Frandsen, H. L. (Intern), Dlouhy, I. (Ekstern), Molin, S. (Intern), Cannio, M. (Ekstern), Hjelm, J. (Intern), Hendriksen, P. V. (Intern)
Pages: 250–253
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Materials Letters
Volume: 162
ISSN (Print): 0167-577X
Ratings:
BFI (2018): BFI-level 1
To enhance the Jc of YBa2Cu3O7−X (YBCO) films both in self-field and under magnetic field, an effective strategy is to introduce artificial pinning centers and keep a good YBCO matrix at the same time. Here, we propose a new dopant:
LaAlO3 (LAO), based on its chemical stability and small mismatch toward YBCO. A series of YBCO films with different LAO doping contents was fabricated on LAO single-crystal substrates by metal organic deposition. We observed by X-ray diffractometer measurements and scanning electron microscopy observations that although a large amount of LAO is added, YBCO still keeps a good epitaxial growth relationship with LAO. Compared with a pure YBCO film, the Jc value of a 5.0% LAO-doped sample is enhanced more than three times in self-field 77 K and seven times at 77 K and 1.5 T, respectively. These results indicate that LAO doping can effectively enhance the Jc of YBCO films both in self-field and in applied magnetic fields.

General information
State: Published
Organisations: Electrofunctional materials, Department of Energy Conversion and Storage
Authors: Xu, Y. (Ekstern), Suo, H. (Ekstern), Yue, Z. (Intern), Grivel, J. (Intern), Liu, M. (Ekstern)
Number of pages: 4
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: IEEE Transactions on Applied Superconductivity
Volume: 26
Issue number: 3
Article number: 6602804
ISSN (Print): 1051-8223
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 1.45 SJR 0.408 SNIP 0.962
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.42 SJR 0.398 SNIP 1.145
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.403 SNIP 1.06 CiteScore 1.27
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.478 SNIP 1.13 CiteScore 0.83
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.443 SNIP 1.156 CiteScore 1.32
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.555 SNIP 1.274 CiteScore 1.11
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.368 SNIP 1.062 CiteScore 1.16
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.473 SNIP 1.065
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.447 SNIP 1.021
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.884 SNIP 0.981
Scopus rating (2007): SJR 0.629 SNIP 1.093
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 0.734 SNIP 1.05
Joining of ceramic Ba$_{0.5}$Sr$_{0.5}$Co$_{0.8}$Fe$_{0.2}$O$_3$ membranes for oxygen production to high temperature alloys

The possibility of joining dense ceramic BCSF tubular membranes to metal alloys using a silver braze was investigated. Four different alloys (Crofer 22 APU (R), Kanthal APM (R), Haynes 214 (R) and EN 1.4841) were considered and the influence of their oxide scale stability/reactivity and their thermal expansion coefficient on the stability of the final joint was evaluated. Leak tight assemblies were obtained only for steels with a thermal expansion coefficient of $> 16 \times 10^{-6}$ K$^{-1}$ and protective coating. Proof-of-concept oxygen flux measurements up to 830 degrees C were performed on these assemblies, demonstrating the functionality of the developed hot sealing. In addition a simulation of the stresses occurring in the joint assembly during use was performed for different materials and geometries. The obtained results fit well with the experimental findings. (C) 2016 Elsevier B.V. All rights reserved.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Electrofunctional materials, Forschungszentrum Jülich GmbH, Fraunhofer Gesellschaft
Authors: Kiebach, W. (Intern), Engelbrecht, K. (Intern), Kwok, K. (Intern), Molin, S. (Intern), Søgaard, M. (Intern), Niehoff, P. (Ekstern), Schulze-Küppers, F. (Ekstern), Kriegel, R. (Ekstern), Kluge, J. (Ekstern), Hendriksen, P. V. (Intern)
Number of pages: 11
Pages: 11-21
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Membrane Science
Volume: 506
ISSN (Print): 0376-7388
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): SNIP 1.898 SJR 2.4 CiteScore 6.93
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 6.13 SJR 2.087 SNIP 1.731
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.978 SNIP 1.763 CiteScore 5.89
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.436 SNIP 1.924 CiteScore 5.42
Web of Science (2014): Indexed yes
Kinetic Studies on State of the Art Solid Oxide Cells: A Comparison between Hydrogen/Steam and Reformate Fuels

Electrochemical reaction kinetics at the electrodes of Solid Oxide Cells (SOCs) were investigated at 700 °C for two cells with different fuel electrode microstructures as well as on a third cell with a reduced active electrode area. Three fuel mixtures were investigated – hydrogen/steam and reformate fuels hydrogen/carbon-dioxide and hydrogen/methane/steam. It was found that the kinetics at the fuel electrode were exactly the same in both reformates. The hydrogen/steam fuel displayed slightly faster kinetics than the reformate fuels. Furthermore the gas conversion impedance in the hydrogen/steam fuel split into two processes with opposing temperature behavior in the reformate fuels. An 87.5 % reduction in active electrode area diminishes the gas conversion impedance in the hydrogen/steam fuel at high fuel flow rates. In both reformates, the second and third lowest frequency processes merged into a single process as the gas conversion was reduced. The SOC with finer electrode microstructure displayed improved kinetics.
Kinetic Study of the Chemical Vapor Deposition of Tantalum in Long Narrow Channels

A kinetic study of the chemical vapor deposition of tantalum in long narrow channels is done to optimize the industrial process for the manufacture of tantalum coated plate heat exchangers. The developed model fits well at temperatures between 750 and 850 °C, and in the pressure range of 25–990 mbar. According to the model, the predominant tantalum growth species is TaCl3. The temperature is shown to have a pronounced effect on the morphology and rate of deposition of the tantalum and an apparent change in deposition mechanism occurs between 850–900 °C, resulting in the deposition rate at 900 °C being lower than both 850 and 950 °C.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors, Tantaline A/S
Authors: Mugabi, J. A. (Intern), Eriksen, S. (Ekstern), Petrushina, I. (Intern), Christensen, E. (Intern), Bjerrum, N. J. (Intern)
Number of pages: 9
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Advanced Materials Interfaces
Volume: 3
Issue number: 14
ISSN (Print): 2196-7350
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 4.13 SJR 1.796 SNIP 0.785
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.57 SJR 1.545 SNIP 0.876
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.193 SNIP 0.668 CiteScore 2.47
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
BFI (2013): BFI-level 1
Large CZTS Nanoparticles Synthesized by Hot-injection for Thin Film Solar Cells

General information
State: Published
Organisations: Department of Photonics Engineering, Department of Energy Conversion and Storage, Imaging and Structural Analysis, Optical Microsensors and Micromaterials, Nanyang Technological University
Authors: Engberg, S. L. J. (Intern), Mirbagheri, N. (Intern), Simonsen, S. B. (Intern), Lam, Y. M. (Ekstern), Schou, J. (Intern)
Publication date: 2016
Event: Abstract from 2016 E-MRS Spring Meeting and Exhibit, Lille, France.
Main Research Area: Technical/natural sciences
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2016

Laser beam induced current mapping (LBIG) of solar cells

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Organic Energy Materials
Authors: Jørgensen, M. (Intern)
Publication date: 2016

Publication information
Media of output: Video
Original language: English
Publisher: DTU Energy
Main Research Area: Technical/natural sciences
Links:
https://youtu.be/gH4vyC-CUsq

Bibliographical note
Invited talk
Publication: Research - peer-review › Sound/Visual production (digital) – Annual report year: 2016

Lifetime of ALD Al2O3 Passivated Black Silicon Nanostructured for Photovoltaic Applications

Black silicon nano-structures provide significant reduction of silicon surface reflection due to highly corrugated nano-structures with excellent light trapping properties. However, most recent RIE techniques for black silicon nano-structuring have one very important limitation for PV applications – high surface recombination velocity due to intensive plasma ion bombardment of the silicon surface. In an attempt to optimize black silicon for PV applications we develop a mask-less one step reactive ion nano-structuring of silicon with low ion surface damage with reflectance below 0.5%. For passivation purposes we used 37 nm ALD Al2O3 films and conducted lifetime measurements and found 1220 µs and to 4170 µs, respectively, for p- and n-type CZ silicon wafers. Such results are promising results to introduce for black silicon RIE nano-structuring in solar cell process flow.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Department of Micro- and Nanotechnology, Silicon Microtechnology, Nanoprobes, Department of Photonics Engineering, Plasmonics and Metamaterials, Experimental Surface and Nanomaterials Physics
Authors: Plakhotnyuk, M. (Intern), Davidsen, R. S. (Intern), Schmidt, M. S. (Intern), Malureanu, R. (Intern), Stamate, E. (Intern), Hansen, O. (Intern)
Number of pages: 1
Publication date: 2016
Event: Poster session presented at 32nd European Photovoltaic Solar Energy Conference and Exhibition, Munich, Germany.
Main Research Area: Technical/natural sciences
Electronic versions:
Lifetime of Nano-Structured Black Silicon for Photovoltaic Applications

In this work, we present recent results of lifetime optimization for nano-structured black silicon and its photovoltaic applications. Black silicon nano-structures provide significant reduction of silicon surface reflection due to highly corrugated nanostructures with excellent light trapping properties. We applied reactive ion etching technology at -20°C to create nano-structures on silicon samples and obtained an average reflectance below 0.5%. For passivation purposes, we used 37 nm ALD Al2O3 films. Lifetime measurements resulted in 1220 µs and to 4170 µs for p- and n-type CZ silicon wafers, respectively. This is promising for use of black silicon RIE nano-structuring in a solar cell process flow.
Lifetime of Organic Photovoltaics: Status and Predictions

The results of a meta-analysis conducted on organic photovoltaics (OPV) lifetime data reported in the literature is presented through the compilation of an extensive OPV lifetime database based on a large number of articles, followed by analysis of the large body of data. We fully reveal the progress of reported OPV lifetimes. Furthermore, a generic lifetime marker has been defined, which helps with gauging and comparing the performance of different architectures and materials from the perspective of device stability. Based on the analysis, conclusions are drawn on the bottlenecks for stability of device configurations and packaging techniques, as well as the current level of OPV lifetimes reported under different aging conditions. The work is summarized by discussing the development of a tool for OPV lifetime prediction and the development of more stable technologies. An online platform is introduced that will aid the process of generating statistical data on OPV lifetimes and further refinement of the lifetime prediction tool.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Functional organic materials
Number of pages: 17
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Advanced Energy Materials
Volume: 6
Issue number: 2
Article number: 1501208
ISSN (Print): 1614-6832
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 16.78 SJR 8.23 SNIP 2.347
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 12.96 SJR 6.515 SNIP 2.14
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 6.219 SNIP 2.546 CiteScore 14.2
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 6.668 SNIP 2.942 CiteScore 15.27
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 6.006 SNIP 2.949 CiteScore 13.24
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Scopus rating (2012): SJR 5.575 SNIP 2.181 CiteScore 9.64
ISI indexed (2012): ISI indexed no
ISI indexed (2011): ISI indexed no
Web of Science (2011): Indexed yes
Original language: English
DOIs: 10.1002/aenm.201501208
Source: PublicationPreSubmission
Source-ID: 118364810
Publication: Research - peer-review › Journal article – Annual report year: 2015

Link between intermittent electrical energy sources and district heating sector
Energy has always been one of the key challenges in planning of societies' development worldwide. The COP conference in Paris in December 2015 has shown unprecedented mutual understanding of harmful consequences climate change can cause. Integrating power and heating sectors in an efficient way is an important step towards achieving the goals of the agreement in a cost-efficient way.
Localized Carbon Deposition in Solid Oxide Electrolysis Cells Studied By Multiphysics Modeling

Modeling for optimizing performance has attracted substantial research efforts in the last twenty years with special focus on solid oxide fuel cells (SOFCs). However, limited amount of the modeling work has been focused on the solid oxide electrolysis cell (SOEC) operation mode and even less on degradation issues connected to SOEC operation. Despite the similarities between the two operation modes, the different operating voltage ranges and the gradients involved influence the long-term degradation and performance in different ways.

Long-term operation of a solid oxide cell stack for coelectrolysis of steam and CO₂

High temperature electrolysis based on solid oxide electrolysis cells (SOECs) is a promising technology for production of synthetic fuels. The SOEC units can be used for co-electrolysis of steam and CO₂ to produce synthesis gas (syngas,
CO+H2), which can be further processed to a variety of synthetic fuels such as methane, methanol or DME. Previously we have reported electrolysis operation of solid oxide cell stacks for periods up to about 1000 hours. In this work, operation of a Haldor Topsoe 8-cell stack (stack design of 2014) in co-electrolysis mode for 6000 hours is reported. The stack consists of Ni/YSZ electrode supported SOEC cells with a footprint of 12X12 cm2. The co-electrolysis operation was carried out by supplying a mixture of 45 % CO2 + 45 % H2O + 10 % H2 to the stack operating with a fixed conversion of 39 % for steam and CO2. The stack was operated at different conditions. Initial operation at 700 oC and -0.25 A/cm2 lasted for only 120 hours due to severe degradation of the bottom cell. Regaining the stack performance was realized by increasing the operation temperature to 750 oC. After reactivation, the stack showed negligible degradation at 750 oC and -0.25 A/cm2 and about 1.4 %/1000 h performance degradation at 750 oC and -0.5 A/cm2. This study demonstrates feasibility of long-term co-electrolysis operation via SOEC stacks and of careful temperature variation as a tool to regain the stack performance.

Long-Term Stability of Anode-Supported Solid Oxide Fuel Cells with a Co-Sintered Cathode Backbone and Infiltrated La0.95Co0.4Ni0.6O3 (LCN) Electro-Catalyst

Infiltration is a fabrication method that is offering potentially significant improvements in cell performance at reduced materials and fabrication costs, especially when combined with co-sintering. However, important questions regarding the long-term performance and microstructural stability of infiltrated electrodes, as well as the mechanical properties of such electrodes have remained unanswered.

Low cost porous MgO substrates for oxygen transport membranes

This paper delineates the fabrication of porous magnesium oxide (MgO) ceramics with high porosity and gas permeability by warm pressing using pre-calcined MgO powder and fugitive pore former (combination of graphite and polymethyl methacrylate). Effect of pore former on the microstructure development of porous MgO ceramic substrates was subjected to investigation. The resultant microstructure consisted of large spherical and elongated pores with small interconnecting pores. The total porosity (55%), mean pore neck size (0.65 μm), and the associated gas permeability (4–4.5×10−15 m2) of
MgO substrates were measured and correlated. Economic analysis of the MgO substrates was performed and it was found that MgO was much cheaper compared to perovskite and fluorite materials.
Low temperature processed MnCo$_2$O$_4$ and MnCo$_{1.8}$Fe$_{0.2}$O$_4$ as effective protective coatings for solid oxide fuel cell interconnects at 750 °C

In this study two materials, MnCo2O4 and MnCo1.8Fe0.2O4 are studied as potential protective coatings for Solid Oxide Fuel Cell interconnects working at 750 °C. First powder fabrication by a modified Pechini method is described followed by a description of the coating procedure. The protective action of the coating applied on Crofer 22 APU is evaluated by following the area specific resistance (ASR) of the scale/coating for 5500 h including several thermal cycles. The coating is prepared by brush painting and has a porous structure after deposition. Post mortem microstructural characterization performed on the coated samples shows good protection against chromium diffusion from the chromia scale ensured by a formation of a dense reaction layer. This study shows, that even without high temperature sintering and/or reactive sintering it is possible to fabricate protective coatings based on MnCo spinels.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Gdansk University of Technology, Jilin University
Authors: Molin, S. (Intern), Jasinski, P. (Ekstern), Mikkelsen, L. (Intern), Zhang, W. (Ekstern), Chen, M. (Intern), Hendriksen, P. V. (Intern)
Number of pages: 11
Pages: 408-418
Publication date: 2016
Main Research Area: Technical/natural sciences
LSCF fibers for IT-SOFCs applications: synthesis and morphological analysis

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Fundamental Electrochemistry, University of Genoa
Authors: Enrico, A. (Ekstern), Zhang, W. (. (Intern), Traulsen, M. L. (Intern), Aliakbarian, B. (Ekstern), Lagazzo, A. (Ekstern), Botter, R. (Ekstern), Perego, P. (Ekstern), Costamagna, P. (Ekstern), Holtappels, P. (Intern)
Number of pages: 1
Publication date: 2016
Event: Abstract from ELectrospinning for ENergy Conference, Montpellier, France.
Main Research Area: Technical/natural sciences
Electronic versions:
elen2016_EnricoAnna_vers.1.pdf
Publication: Research › Conference abstract for conference – Annual report year: 2016
Magnetocaloric materials and first order phase transitions

This thesis studies the first order phase transitions of the magnetocaloric materials La$_{0.67}$Ca$_{0.33}$MnO$_3$ and La(Fe,Mn,Si)$_{13}H_2$, trying to overcome challenges that these materials face when applied in active magnetic regenerators. The study is done through experimental characterization and modelling of the properties of such materials. The experimental characterization of these materials is done through various different methods, such as X-ray diffraction, magnetometry, calorimetry, direct measurements of entropy change, capacitance dilatometry, scanning electron microscopy, energy-dispersive X-ray spectrometry and magnetocaloric regenerative tests. The magnetic, thermal and structural properties obtained from such measurements are then evaluated through different models, i.e. the Curie-Weiss law, the Bean-Rodbell model, the free electron model and the Debye model. The measured magnetocaloric properties of La$_{0.67}$Ca$_{0.33}$MnO$_3$ shows a paradoxical behavior; the material shows features of both a first order phase transition and of a second order one. Identities as shift of the heat capacity peak and an asymmetric growth of of the entropy change with magnetic field would describe this material transition as a first order one. However, the material did not present any signs of intrinsic hysteresis, a feature common in first order transitions. This is attributed to a chemical distribution in this first order phase transition material that can lead to a smearing of the transition and the hysteresis, and such effect is observed through modelling. Moreover, inverse susceptibility measurements showed what could be evidences of magnetic polarons being formed in the paramagnetic phase of the material. The origin of the first order transition seems to be due to the magnetoelastic coupling observed through isothermal magnetostriction and dilatometric measurements. Although the Bean-Rodbell model has described with a good agreement the entropy change, hysteresis, magnetization and heat capacity, it has failed to describe the isothermal magnetostriction. It is suggested that such failure could be related to different factors that might influence constructively to each other: (i) the model assumes localized magnetic moments, while this material presents a double exchange interaction; (ii) the model assumes a temperature and field independent bulk modulus, which literature has shown that is not the case; and (iii) the approximation of the cluster being temperature and field independent is exaggerated and perhaps cannot be taken. A series of La(Fe,Mn,Si)$_{13}H_2$ with slightly changes in the composition is also evaluated here. This material may present a second order phase transition for large content of Mn and Si, which will become a first order one as the Mn and Si content decreases. The material also presents a volume change, which also increases as Mn and Si content decreases, which in return may lead to detrimental mechanical stability of the material during application. The shift of the orderliness from second to first order transition is observed through heat capacity, magnetization and entropy change measurements. By measuring bulky particles (with a particle size in the range of 500-1000 μm) of La(Fe,Mn,Si)$_{13}H_2$ with first order phase transition, it was possible to observe very sharp transitions. This is not the case for finer ground particles which show a smooth transition, as if it was second order. Although this behavior has been explained in the literature as an artefact due to the inclusion of defects when grinding the material, here it is proposed a different explanation given the evidences. Firstly, it is argued that the material is brittle and insertion of defects through grinding is unlikely. Secondly, it is observed through entropy change measurements that a bulky particle has a larger entropy change. However, the particle cracks and separates into several particles due to stresses generated during the transition, which are related to the volume change. After this effect, if the entropy change is remeasured it shows very similar behavior to measurements of ground particles. Therefore, the results suggests that defects inserted through grinding is probably not the case. To explain such behavior, in this thesis it is proposed that slightly differences in the composition throughout the sample may lead to a Curie temperature distribution. This in return would lead to different regions of the sample undergoing the transition in different temperatures. However, given the polycrystallinity of the material, the crystallites with different Curie temperatures will be volumetric constrained until enough energy is given to the system and the whole bulky particle undergoes the transition. This explains why bulky particles have a sharp transition and ground particle have a smoother one; the latter is much less volumetric constrained than the former. An outcome of such behavior is observed as strain development during the phase transition; this strain was calculated applying the Williamson-Hall method. The strain development is much more significant in the ferromagnetic phase than in the paramagnetic one, which is attributed to the weakening of the magnetic interactions as the ferromagnetic phase approach the transition. This is speculated as a decrease of the bulk modulus of the ferromagnetic phase as the temperature increases. The paramagnetic phase, however, is expected to have a relatively constant bulk modulus as there is no magnetic interactions. When observing the microscopy images, they show that cracks are usually somehow connected to a minor La-rich secondary phase observed as inclusions in the grain boundaries. It is argued that this phase is the only brittle and hard phase that does not present a volume change. Therefore the decrease of this phase, however low content it is, could lead to an improvement in the mechanical stability of the material during application. Finally the Bean-Rodbell model is applied to the describe the volumetric behavior observed through X-ray measurements as a function of the temperature. The model describes with good agreement the volume discontinuity across the phase transition, and the superimposed distribution of Curie temperature can describe well the paramagnetic growth as the transition occurs. However, the model over-predicts the thermal hysteresis and under-predicts the shift of the transition temperature with magnetic field.

General information
State: Published
Organisations: Electrofunctional materials, Department of Energy Conversion and Storage
Authors: Neves Bez, H. (Intern), Bahl, C. (Intern), Nielsen, K. K. (Intern), Smith, A. (Intern)
Number of pages: 170
Publication date: 2016

Publication information
Publisher: Department of Energy Conversion and Storage, Technical University of Denmark
Original language: English
Magneto-elastic coupling in La(Fe, Mn, Si)$_{13}$H$_y$ within the Bean-Rodbell model

First order magnetic phase transition materials present a large magnetocaloric effect around the transition temperature, where these materials usually undergo a large volume or structural change. This may lead to some challenges for applications, as the material may break apart during field change, due to high internal stresses. A promising magnetocaloric material is La(Fe, Mn, Si)$_{13}$H$_y$, where the transition temperature can be controlled through the Mn amount. In this work we use XRD measurements to evaluate the temperature dependence of the unit cell volume with a varying Mn amount. The system is modelled using the Bean-Rodbell model, which is based on the assumption that the spin-lattice coupling depends linearly on the unit cell volume. This coupling is defined by the model parameter $\eta$, where for $\eta > 1$ the material undergoes a first order transition and for $\eta \leq 1$ a second order transition. We superimpose a Gaussian distribution of the transition temperature with a standard deviation $\sigma_T$, in order to model the chemical inhomogeneity. Good agreement is obtained between measurements and model with values of $\eta \sim 1.8$ and $\sigma(T) = 1.0$ K.
Manufacture, installation and decommissioning of organic solar cell parks

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Organic Energy Materials
Authors: Søndergaard, R. R. (Intern)
Publication date: 2016

Manufacturing of a LaNiO$_3$ composite electrode for oxygen evolution in commercial alkaline water electrolysis

The LaNiO$_3$ perovskite was chosen for incorporation into a nickel matrix in order to obtain a metallic composite electrode suitable for improving the oxygen evolution reaction (OER) in commercial water electrolysis at elevated temperature. The manufactured LaNiO$_3$ + Ni composite coatings were deposited in a Watts type nickel electrolyte in a specially designed beaker with continuous particle circulation. Activity of the composite coatings was evaluated using cyclic voltammetry (CV), electrochemical impedance spectroscopy (EIS) and anodic potentiodynamic polarization measurements. The obtained results were compared to a non-catalysed Watts nickel reference sample and the electrochemical measurements confirmed that the coating decreased the OER overpotential by 70 mV. XRD furthermore revealed that a LaNiO$_3$ + Ni composite structure was obtained. Conventional alkaline water electrolysis was carried out at a temperature of 120 °C and a current densities of 0.2 and 0.8 A cm$^{-2}$. Scanning Electron Microscopy (SEM), Energy Dispersive X-ray Spectroscopy (EDS) and X-ray Diffraction (XRD) were used for characterization of the morphology.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors, Department of Mechanical Engineering, Materials and Surface Engineering, Siemens (DK)
Authors: Egelund, S. (Ekstern), Caspersen, M. (Ekstern), Nikiforov, A. V. (Intern), Møller, P. (Intern)
Number of pages: 9
Pages: 10152-10160
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Volume: 41
Issue number: 24
ISSN (Print): 0360-3199
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 4.1 SJR 1.116 SNIP 1.267
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.74 SJR 1.145 SNIP 1.315
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.27 SNIP 1.314 CiteScore 3.46
Web of Science (2015): Indexed yes
Marginal Generation Technology in the Chinese Power Market towards 2030 Based on Consequential Life Cycle Assessment

Electricity consumption is often the hotspot of life cycle assessment (LCA) of products, industrial activities, or services. The objective of this paper is to provide a consistent, scientific, region-specific electricity-supply-based inventory of electricity generation technology for national and regional power grids. Marginal electricity generation technology is pivotal in assessing impacts related to additional consumption of electricity. China covers a large geographical area with regional supply grids; these are arguably equally or less integrated. Meanwhile, it is also a country with internal imbalances in regional energy supply and demand. Therefore, we suggest an approach to achieve a geographical subdivision of the Chinese electricity grid, corresponding to the interprovincial regional power grids, namely the North, the Northeast, the East, the Central, the Northwest, and the Southwest China Grids, and the China Southern Power Grid. The approach combines information from the Chinese national plans on for capacity changes in both production and distribution grids, and knowledge of resource availability. The results show that nationally, marginal technology is coal-fired electricity generation, which is the same scenario in the North and Northwest China Grid. In the Northeast, East, and Central China...
Grid, nuclear power gradually replaces coal-fired electricity and becomes the marginal technology. In the Southwest China Grid and the China Southern Power Grid, the marginal electricity is hydropower towards 2030.

**General information**

State: Published
Organisations: Department of Energy Conversion and Storage, Chinese Research Academy of Environmental Sciences, Aalborg University
Authors: Zhao, G. (Intern), Guerrero, J. M. (Forskerdatabase), Pei, Y. (Ekstern)
Number of pages: 14
Publication date: 2016
Main Research Area: Technical/natural sciences

**Publication information**

Journal: Energies
Volume: 9
Issue number: 10
Article number: 788
ISSN (Print): 1996-1073
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 3.11 SJR 0.67 SNIP 1.34
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.5 SJR 0.662 SNIP 1.106
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.785 SNIP 1.399 CiteScore 2.87
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 0.844 SNIP 1.565 CiteScore 2.66
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.613 SNIP 1.331 CiteScore 2.29
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.852 SNIP 1.53 CiteScore 2.46
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.651 SNIP 1.396 CiteScore 2.24
ISI indexed (2011): ISI indexed no
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.302 SNIP 0.734
Original language: English
Marginal technology, Power grid, Consequential life cycle assessment, China
Electronic versions:
Marginal_Generation_Technology_in_the_Chinese_Power_Market_towards_2030_Based_on_Consequential_Life_Cycle_Assessment.pdf
DOIs: 10.3390/en9100788

**Bibliographical note**

This is an open access article distributed under the Creative Commons Attribution License (CC BY 4.0).
Source: PublicationPreSubmission
Source-ID: 126147343
Publication: Research - peer-review › Journal article – Annual report year: 2016
Material transfer in Pulsed Laser Deposition of the solar cell materials Cu₂SnS₃ and Cu₂ZnSnS₄.

General information
State: Published
Organisations: Department of Photonics Engineering, Photovoltaic Materials and Systems, Department of Physics, Experimental Surface and Nanomaterials Physics, Silicon Microtechnology, DTU Danchip, Department of Energy Conversion and Storage, Electrofunctional materials, Department of Micro- and Nanotechnology
Authors: Cazzaniga, A. C. (Intern), Canulescu, S. (Intern), Crovetto, A. (Intern), Ettlinger, R. B. (Intern), Pryds, N. (Intern), Hansen, O. (Intern), Schou, J. (Intern)
Number of pages: 1
Publication date: 2016
Event: Abstract from Annual Meeting of the Danish Physical Society, Middelfart, Denmark.
Main Research Area: Technical/natural sciences
Electronic versions:
abstract_DFS_2016_Andcan.pdf

Mechanical Characterization of Energy Materials at DTU Energy
Due to the ever growing demand for sustainable energy alternatives, increasing the efficiency as well as reliability of energy conversion and storage technologies is becoming paramount challenge for the research community in the field. To achieve this, the innovation of new material systems should go hand in hand with understanding and improving their mechanical reliability at operational conditions. With this regard, DTU energy has a dedicated team and facilities working on characterization of metallic as well as ceramic materials used in energy conversion and storage technologies. The poster presents the unique capabilities in the department including high throughput and high temperature strength and deformational behavior characterization of materials in a controlled atmosphere. The characterization techniques mainly focus on materials being developed to be used in solid oxide fuel or electrolysis cells, oxygen or gas membranes, etc.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors
Authors: Tadesse Molla, T. (Intern), Han, L. (Intern), Frandsen, H. L. (Intern)
Number of pages: 1
Publication date: 2016
Main Research Area: Technical/natural sciences
Links:
http://www.sustain.dtu.dk/

Bibliographical note
Sustain Abstract M-18
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2016

Mechanical Properties of a Library of Low-Band-Gap Polymers
The mechanical properties of low-band-gap polymers are important for the long-term survivability of roll to-roll processed organic electronic devices. Such devices, e.g., solar cells, displays, and thin-film transistors, must survive the rigors of roll-to-roll coating and also thermal and mechanical forces in the outdoor environment and in stretchable and ultraflexible form factors. This paper measures the stiffness (tensile modulus), ductility (crack-onset strain), or both of a combinatorial library of 51 low-band-gap polymers. The purpose of this study is to systematically screen a library of low-band-gap polymers to better understand the connection between molecular structures and mechanical properties in order to design conjugated polymers that permit mechanical robustness and even extreme deformability. While one of the principal conclusions of these experiments is that the structure of an isolated molecule only partially determines the mechanical properties another important codeterminant is the packing structure some general trends can be identified. (1) Fused rings tend to increase the modulus and decrease the ductility. (2) Branched side chains have the opposite effect. Despite the rigidity of the molecular structure, the most deformable films can be surprisingly compliant (modulus >= 150 MPa) and ductile (crack-onset strain

General information
State: Published
Mg/O2 Battery Based on the Magnesium-Aluminum Chloride Complex (MACC) Electrolyte

Mg/O2 cells employing a MgCl2/AlCl3/DME (MACC/DME) electrolyte are cycled and compared to cells with modified Grignard electrolytes, showing that performance of magnesium/oxygen batteries depends strongly on electrolyte composition. Discharge capacity is far greater for MACC/DME-based cells, while rechargeability in these systems is severely limited. The Mg/O2-MACC/DME discharge product comprises a mixture of Mg(ClO4)2 and MgCl2, with the latter likely formed from slow decomposition of the former. The presence of Cl in these compounds suggests that the electrolyte participates in the cell reaction or reacts readily with the initial electrochemical products. A rate study suggests that O2 diffusion in the electrolyte limits discharge capacities at higher currents. Formation of an insulating product film on the positive electrodes of Mg/O2-MACC/DME cells following deep discharge increases cell impedance substantially and likely explains the poor rechargeability. An additional impedance rise consistent with film formation on the Mg negative electrode suggests the presence of detrimental O2 crossover. Minimizing O2 crossover and bypassing charge transfer through the discharge product would improve battery performance.
Modeling of active magnetic regenerators and experimental investigation of passive regenerators with oscillating flow

This thesis presents numerical modeling of active magnetic regenerator (AMR) and passive regenerator tests with oscillating flow. The work serves to investigate and improve the understanding of emerging concepts and technologies in the area of magnetic refrigeration. The discretization scheme of a one dimensional (1D) AMR model is improved for decreasing spurious temperature oscillations in the numerical solution. This transient AMR model is further modified for simulating tapered regenerators, heat loss through the housing wall and regenerators using mixed materials. Magnetocaloric materials (MCM) with a first or second order phase transition (FOPT or SOPT) exhibit different characteristics in isothermal entropy change $\Delta S_{iso}$, adiabatic temperature change $\Delta T_{ad}$ and temperature dependence of the magnetocaloric effect (MCE). A theoretical study quantifies the impact of these parameters, showing that all of them are equally important. Based on measured magnetocaloric properties of $\text{La(Fe,Mn,\text{Si})}_{13}\text{H}_y$ and Gd, a thorough investigation on how to layer typical FOPT or SOPT materials is implemented. For those regenerators, the sensitivity to the working temperature and the Curie temperature variation is evaluated. A concept of mixing FOPT and SOPT materials is also investigated. Furthermore, the entropy production rates due to insufficient heat transfer, viscous dissipation and
axial conduction, as well as the total entropy production rate, are calculated and compared for analyzing different loss mechanisms and optimizing AMRs. The impacts of the heat loss through the regenerator housing and the dead volume are also quantified. A multiparameter optimization reveals the optimal dimensions and operating parameters for different regenerator geometries. In order to evaluate different regenerator geometries, including the emerging epoxy bonded bed and different heat transfer fluids, a passive regenerator test apparatus is constructed and an experimental investigation is presented. The flow and heat transfer characteristics of different regenerators are estimated by presenting the measured and deduced indicators, including the pressure drop, friction factor, effectiveness, heating power and overall Nusselt number. Finally, based on the research in this thesis, the perspectives and some suggestions for the future work are given.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, University of Southern Denmark
Authors: Lei, T. (Intern), Engelbrecht, K. (Intern), Nielsen, K. K. (Intern), Veje, C. T. (Ekstern)
Number of pages: 270
Publication date: 2016

Publication information
Publisher: Department of Energy Conversion and Storage, Technical University of Denmark
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
Modeling_of_active_magnetic_regeneration.pdf

Relations
Projects:
Modeling of active magnetic regenerators and experimental investigation of passive regenerators with oscillating flow
Publication: Research › Ph.D. thesis – Annual report year: 2016

Modeling of transport phenomena in battery cathode materials
General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, Technical University of Denmark
Authors: García Lastra, J. M. (Intern), Mekonnen, Y. S. (Intern), Loftager, S. (Intern), Melander, M. (Intern), Mathiesen, N. R. (Ekstern), Christensen, R. (Intern), Vegge, T. (Intern)
Number of pages: 1
Publication date: 2016
Main Research Area: Technical/natural sciences
Electronic versions:
ABSTRACT_Garcia_Lastra_The_Hague.pdf
Source: PublicationPreSubmission
Source-ID: 128083393
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2016

Modelling transition towards sustainable transportation sector
General information
State: Published
Organisations: Centre for IT-Intelligent Energy Systems in Cities, Department of Energy Conversion and Storage
Authors: Dominkovic, D. F. (Intern), Bačeković, I. (Ekstern), Myrdal, J. S. G. (Intern), Pedersen, A. S. (Intern), Krajačić, G. (Ekstern)
Number of pages: 14
Publication date: 2016

Publication information
Media of output: PowerPoint
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
Modelling_transition_towards_sustainable_transportation_sector.pdf
Modelling Transition Towards Sustainable Transportation Sector

In a transition towards 100% renewable energy system, transportation sector is rarely dealt with using the holistic approach and measuring its impact on the whole energy system. Furthermore, solutions for power and heat sectors are clearer, it is a tendency of the researchers to focus on the latter two energy sectors. In order to deal with the raised issue, authors of this paper developed a methodology for calculation of the transition towards sustainable transport sector, focusing on the solutions that are already available. Furthermore, as a part of the model, a detailed mapping of resources needed has been carried out for each of the alternatives. It was shown that the electrification of the transportation sector is a crucial point in transition, while for the transport modes that cannot be electrified, or shifted to different transportation modes, four alternatives were defined: synthetic fuels, biofuels, hydrogen and synthetic fuels utilizing excess intermittent electricity generation. Results showed that the 72.3% of the fossil fuel demand in transportation sector of the European Union (EU) can be replaced by electricity demand, reducing final energy demand in transportation sector for 50.6% or 2,051 TWh. All the alternatives for the non-electrified part of transportation suffer from the low well-to-wheel efficiency, resulting in a significant amount of additional resources needed. Replacing remaining part of the fossil fuels by biofuels led to the increase of demand for biomass on EU level equal to 3,069 TWh, which is extremely challenging to meet in the future in a sustainable way. In the case of synthetic fuel production as an alternative, additional electricity demand was calculated to be 2,775 TWh, which is approximately 90% of the total electricity demand of the EU for the year 2013. Hence, authors argued that due to the enormous additional demand for scarce resources for producing alternatives to the fossil fuels, concepts such as car sharing, induction charging on highways, promotion of bicycling and public transportation should be assessed in more detailed way in order to bring additional energy savings in the sector.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Aalborg University, University of Zagreb
Authors: Dominkovic, D. F. (Intern), Bačeković, I. (Ekstern), Myrdal, J. S. G. (Intern), Pedersen, A. S. (Intern), Krajačić, G. (Ekstern)
Pages: 154-154
Publication date: 2016
Nanocomposite YSZ-NiO Particles with Tailored Structure Synthesized in a Two-Stage Continuous Hydrothermal Flow Reactor

The increasing amount of fluctuating electricity generation from renewable sources requires a flexible energy system and storage technologies to ensure that energy services can be covered in a stable and affordable manner. In order to become truly independent from fossil fuels, increasing the performance of energy storage and conversion devices such as fuel cells, electrolyzers and batteries is important. One promising approach to further improve these devices is the use of carefully structured nanosized materials. Nano-composite particles combining different materials in advanced geometries like core-shell structures or surface decorated particles could exhibit better performance compared with single phase materials. To obtain such advanced structures is the aim of the ProEco project (www.proeco.dk). In this project, a two-stage continuous reactor is built and used to synthesize such nano-composites.

Here we report on the design of the two-stage continuous hydrothermal flow synthesis reactor and first results on obtaining structured nano-composite consisting of yttria-stabilized zirconia (YSZ) and NiO materials. These materials are commonly applied in the fuel electrodes of today’s state-of-the-art solid oxide fuel and electrolysis cells. The prepared particles were characterized by X-ray powder diffraction, (high resolution) transmission electron microscopy, scanning tunnel transmission microscopy and Raman spectroscopy in order to determine crystal structure, particle size, surface morphology and element distribution.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Imaging and Structural Analysis, Atomic scale modelling and materials
Authors: Zielke, P. (Intern), Xu, Y. (Intern), Kiebach, W. (Intern), Simonsen, S. B. (Intern), Norby, P. (Intern), Hendriksen, P. V. (Intern)
Publication date: 2016
Conference: PRiME 2016/230th ECS Meeting, Honolulu, United States, 02/10/2016 - 02/10/2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Electrochemical Society. Meeting Abstracts (Online)
Volume: MA2016-02
Article number: 2953
ISSN (Print): 2151-2043
Original language: English
Links:
http://ma.ecsdl.org.proxy.findit.dtu.dk/content/MA2016-02/39/2953
Publication: Research - peer-review › Conference abstract in journal – Annual report year: 2016

Nanoconfinement of LiBH₄ for High Ionic Conductivity in Lithium Ion Batteries

Efficient energy conversion and storage is crucial for development of systems based on renewable energy sources. For electricity storage, Li-ion batteries are commonly used in electronics devices but require many improvements to obtain longer life-time and higher energy densities. The current use of organic liquids and gels electrolytes limits these improvements because of lithium dendrites formation, reducing the lifetime of the battery and which can possibly be hazardous due to risks of short circuits.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials
Authors: Lefevr, J. E. A. (Intern), Das, S. (Intern), Blanchard, D. (Intern)
Pages: 177-177
Publication date: 2016

Host publication information
Title of host publication: ISPE-XV, Uppsala 15-19th August 2016
Article number: P52
Main Research Area: Technical/natural sciences
Electronic versions:
Nanoconfinement_of_LiBH4_for_High_Ionic_Conductivity_in_Lithium_Ion_Batteries.pdf
Nanostructured materials for solid-state hydrogen storage: A review of the achievement of COST Action MP1103

In the framework of the European Cooperation in Science and Technology (COST) Action MP1103 Nanostructured Materials for Solid-State Hydrogen Storage were synthesized, characterized and modeled. This Action dealt with the state of the art of energy storage and set up a competitive and coordinated network capable to define new and unexplored ways for Solid State Hydrogen Storage by innovative and interdisciplinary research within the European Research Area. An important number of new compounds have been synthesized: metal hydrides, complex hydrides, metal halide amines and amidoboranes. Tuning the structure from bulk to thin film, nanoparticles and nanoconfined composites improved the hydrogen sorption properties and opened the perspective to new technological applications. Direct imaging of the hydrogenation reactions and in situ measurements under operando conditions have been carried out in these studies. Computational screening methods allowed the prediction of suitable compounds for hydrogen storage and the modeling of the hydrogen sorption reactions on mono-, bi-, and three-dimensional systems. This manuscript presents a review of the main achievements of this Action. © 2016 Hydrogen Energy Publications LLC. Published by Elsevier Ltd. All rights reserved.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, Swiss Federal Institute of Technology, University of New South Wales, Universidad Autónoma de Madrid, University of Antwerp, University of Zagreb, Uppsala University, National Centre for Scientific Research "Demokritos", Helmholtz-Zentrum Geesthacht Centre for Materials and Coastal Research, CNRS-UPEC, Delft University of Technology, Max Planck Institute for Intelligent Systems, ENEA Centro Ricerche Casaccia, Università di Bologna, University of Belgrade, Université Catholique de Louvain, Utrecht University, Aarhus University, Swiss Federal Laboratories for Materials Testing and Research
Number of pages: 25
Pages: 14404-14428
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Volume: 41
Issue number: 32
ISSN (Print): 0360-3199
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 4.1 SJR 1.116 SNIP 1.267
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.74 SJR 1.145 SNIP 1.315
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.27 SNIP 1.314 CiteScore 3.46
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
New Hypothesis for SOFC Ceramic Oxygen Electrode Mechanisms

A new hypothesis for the electrochemical reaction mechanism in solid oxide cell ceramic oxygen electrodes is proposed based on literature including our own results. The hypothesis postulates that the observed thin layers of SrO-La\textsubscript{2}O\textsubscript{3} on top of ceramic perovskite and other Ruddlesden-Popper structured electrode materials are sufficiently electron and oxygen ion conducting to provide reaction sites despite that the bulk phase of such an oxide layer is insulating. We claim that a few nanometer thin layer of mixed SrO-La\textsubscript{2}O\textsubscript{3} that contains some dissolved transition metal and some impurities plus two space charge layers – one towards the gas phase and the other towards the perovskite – will be sufficiently oxide ion (vacancy) and electron conducting to support the electrode process. We also present some considerations about a possible mechanism of improved electrodes.

General information

State: Published
Organisations: Department of Energy Conversion and Storage, Fundamental Electrochemistry, Applied Electrochemistry, Imaging and Structural Analysis
New Insights into the Creation of High-Mobility Two-Dimensional Electron Gas at Oxide Interfaces: Control of Interfacial Redox Reactions by an Electron Sink

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, University of British Columbia, Canadian Light Source, Chinese Academy of Sciences
Authors: Chen, Y. (Intern), Green, R. (Ekstern), Trier, F. (Intern), Christensen, D. V. (Intern), Sutarto, R. (Ekstern), He, F. (Ekstern), von Soosten, M. (Intern), Zhang, Y. (Ekstern), Linderoth, S. (Intern), Pryds, N. (Intern)
Number of pages: 1
Publication date: 2016
Event: Abstract from 23rd International Workshop on Oxide Electronics, Nanjing, China.
Ni/YSZ electrodes structures optimized for increased electrolysis performance and durability

Cermet Ni/YSZ electrodes are the most commonly applied fuel electrode for solid oxide cells (SOC) both when targeting solid oxide fuel cell (SOFC) applications and when used as solid oxide electrolysis cell (SOEC). In this work we report on the correlation between initial Ni/YSZ microstructure and the resulting electrochemical performance both initially and during long-term electrolysis testing at high current density and high p(H2O) inlet. Especially, this work focuses on microstructure optimization to hinder Ni mobility and migration during long-term operation and illustrates the key-role of electrode over-potential on the degradation of the Ni/YSZ electrodes in SOEC. We find that for long-term stability for electrolysis at high current densities and high p(H2O) the as-produced NiO/YSZ precursor electrode should be: 1) As dense as possible, 2) as fine particle and pore sized as possible and 3) the three phases (Ni, YSZ and pore phase) shall be size-matched and well-dispersed. Applying such microstructure optimized Ni/YSZ electrode we show SOEC test results with long-term degradation rate as low as 0.3-0.4%/kh at - 1 A/cm², 800 °C and inlet gas mixture of p(H2O)/p(H2):90/10. This enables SOEC operation of such cell for more than 5 years below thermo-neutral potential at these operating conditions.
Scopus rating (2011): SJR 1.376 SNIP 1.615 CiteScore 2.96
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.46 SNIP 1.498
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.508 SNIP 1.483
Web of Science (2009): Indexed yes
Scopus rating (2008): SJR 1.515 SNIP 1.617
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.292 SNIP 1.384
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.239 SNIP 1.541
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.093 SNIP 1.423
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.18 SNIP 1.55
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.473 SNIP 1.389
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 1.253 SNIP 1.36
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 1.121 SNIP 1.213
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 1.161 SNIP 1.312
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 1.08 SNIP 1.254
Original language: English
Solid oxide electrolysis cells, Ni/YSZ electrode, Microstructure, Electrochemical impedance spectroscopy, Performance, Durability
Electronic versions:
SSI_2016_190_Manuscript_Changes_NOT_Highlighted_AnneHauch_20160606.pdf. Embargo ended: 12/06/2018
DOIs:
10.1016/j.ssi.2016.06.003
Source: FindIt
Source-ID: 2305613605
Publication: Research - peer-review › Journal article – Annual report year: 2016

Non-Platinum Oxygen Reduction Catalysts. From Crystalline to Molecular Moieties

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors
Authors: Jensen, J. O. (Intern), Hu, Y. (Intern), Zhong, L. (Intern), Pan, C. (Intern), Cleemann, L. N. (Intern), Li, Q. (Intern)
Number of pages: 1
Publication date: 2016
Event: Abstract from 4th International Workshop on Solution Plasma and Molecular Technology (SPM-4), Pilsen, Czech Republic.
Main Research Area: Technical/natural sciences

Bibliographical note
Invited talk
Source: PublicationPreSubmission
Source-ID: 127806199
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2016
Nonuniversal scaling of the magnetocaloric effect as an insight into spin-lattice interactions in manganites

We measure the magnetocaloric effect of the manganite series \( \text{La0.67Ca0.33-xSrxMnO3} \) by determining the isothermal entropy change upon magnetization, using variable-field calorimetry. The results demonstrate that the field dependence of the magnetocaloric effect close to the critical temperature is not given uniquely by the critical exponents of the ferromagnetic-paramagnetic phase transition, i.e., the scaling is nonuniversal. A theoretical description based on the Bean-Rodbell model and taking into account compositional inhomogeneities is shown to be able to account for the observed field dependence. In this way the determination of the nonuniversal field dependence of the magnetocaloric effect close to a phase transition can be used as a method to gain insight into the strength of the spin-lattice interactions of magnetic materials. The approach is shown also to be applicable to first-order transitions.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Secretariat, IT, Electrofunctional materials
Authors: Smith, A. (Intern), Nielsen, K. K. (Intern), Neves Bez, H. (Intern), Bahl, C. (Intern)
Number of pages: 5
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication Information
Journal: Physical Review B
Volume: 94
Issue number: 5
Article number: 054411
ISSN (Print): 2469-9950
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 3.34 SJR 1.604 SNIP 1.04
Web of Science (2017): Indexed yes
Scopus rating (2016): CiteScore 3.16 SJR 2.339 SNIP 1.151
Web of Science (2016): Indexed yes
Scopus rating (2015): SJR 2.377 SNIP 1.13 CiteScore 2.8
Web of Science (2015): Indexed yes
Scopus rating (2014): SJR 2.762 SNIP 1.316 CiteScore 3.3
Web of Science (2014): Indexed yes
Scopus rating (2013): SJR 2.813 SNIP 1.326 CiteScore 3.55
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Scopus rating (2012): SJR 3.173 SNIP 1.378 CiteScore 3.57
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
Scopus rating (2011): SJR 3.326 SNIP 1.423 CiteScore 3.61
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
Scopus rating (2010): SJR 3.318 SNIP 1.447
Web of Science (2010): Indexed yes
Web of Science (2009): Indexed yes
Scopus rating (2008): SJR 2.923 SNIP 1.516
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 2.892 SNIP 1.588
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 2.62 SNIP 1.468
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 2.126 SNIP 1.156
Novel ceramic processing method for substitution of toxic plasticizers

A systematic screening of plasticisers for a polyvinyl butyral based binder system revealed that dibutyl maleate, dibutyl adipate and Pycal 94 are promising and less toxic alternatives to the very harmful but frequently used dibutyl phthalate. Pycal 94 seems especially promising as it unlike the two other candidates did not require a co-plasticiser, such as a polyethylene glycol, thus simplifying the system and reducing the risk of unwanted cross-interactions. An effective and systematic procedure for substitution of the plasticiser, while maintaining chemical compatibility and mechanical properties, was also demonstrated. Incompatible systems were discarded in an initial broad screening while primary systems were further evaluated based on debinding properties, mechanical properties, flow behavior as well as sintering properties of ceramic tapes. The thermomechanical characterization performed on dried drops of binder and their corresponding tapes show strong similarities in the strain/stress profiles, validating the qualitative method used.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science
Authors: Foghmoes, S. P. V. (Intern), Teocoli, F. (Intern), Brodersen, K. (Intern), Klemensø, T. (Intern), Della Negra, M. (Intern)
Number of pages: 9
Pages: 3441-3449
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of the European Ceramic Society
Volume: 36
Issue number: 14
ISSN (Print): 0955-2219
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 3.55 SJR 1.068 SNIP 1.698
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.25 SJR 1.142 SNIP 1.888
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.135 SNIP 1.817 CiteScore 3.03
Web of Science (2015): Indexed yes
Novel high band gap pendant-borylated carbazole polymers with deep HOMO levels through direct $^+$N=B$^-$ interaction for organic photovoltaics

In this communication, we investigate the direct and still conjugated intramolecular $^+$N=B$^-$ interactions in novel high band gap borylated carbazole containing polymers, namely, poly(3,6-(N-di(2,4,6-trimethyl)-phenylboryl-carbazole)-alt-4,8-di(5-(2-ethylhexyl)thiophene-2-yl)benzo[1,2-b:4,5-b'] dithiophene) (P(3,6-BCBDT)) and poly(3,6-(N-di(2,4,6-trimethyl)phenylboryl-carbazole)-alt-3,3'''-didodecyl-2,2':5',2':5'',2'''-quaterthiophene) (P(3,6-BCQT)), which result in ambipolarity, high electron affinity, and deep HOMO levels. The quasi-donor-acceptor nature of the two polymers was confirmed by UV-Vis absorption, electro-chemical property studies, and computer modelling. Band gaps of 2.07 eV for P(3,6-BCBDT) and 2.23 eV for P(3,6-BCQT) were obtained. P(3,6-BCQT) afforded a power conversion efficiency of 1.44%, with a $J_{sc}$ of 4.82 mA cm$^{-2}$, a $V_{oc}$ of 0.79 V and a FF of 37%, and P(3,6-BCBDT) performed better with an efficiency of 3.82%, with a $J_{sc}$ of 8.31 mA cm$^{-2}$, a $V_{oc}$ of 1.0 V based on its low lying HOMO level, and a FF of 45%.
Novel micro-reactor flow cell for investigation of model catalysts using in situ grazing-incidence X-ray scattering

The design, fabrication and performance of a novel and highly sensitive micro-reactor device for performing in situ grazing-incidence X-ray scattering experiments of model catalyst systems is presented. The design of the reaction chamber, etched in silicon on insulator (SOI), permits grazing-incidence small-angle X-ray scattering (GISAXS) in transmission through 10 µm-thick entrance and exit windows by using micro-focused beams. An additional thinning of the Pyrex glass reactor lid allows simultaneous acquisition of the grazing-incidence wide-angle X-ray scattering (GIWAXS). In situ experiments at synchrotron facilities are performed utilizing the micro-reactor and a designed transportable gas feed and analysis system. The feasibility of simultaneous in situ GISAXS/GIWAXS experiments in the novel micro-reactor flow cell was confirmed with CO oxidation over mass-selected Ru nanoparticles.
On Degradation Issues in High-Temperature Electrochemical Devices

General information
State: Published
Organisations: Fundamental Electrochemistry, Department of Energy Conversion and Storage, Forschungszentrum Jülich GmbH
Authors: De Haart, L. (Ekstern), Holtappels, P. (Intern)
Number of pages: 37
Publication date: 2016

On performance limitations and property correlations of Al-doped ZnO deposited by radio-frequency sputtering: Paper

The electrical properties of RF-sputtered Al-doped ZnO are often spatially inhomogeneous and strongly dependent on deposition parameters. In this work, we study the mechanisms that limit the minimum resistivity achievable under different deposition regimes. In a low- and intermediate-pressure regime, we find a generalized dependence of the electrical properties, grain size, texture, and Al content on compressive stress, regardless of sputtering pressure or position on the substrate. In a high-pressure regime, a porous microstructure limits the achievable resistivity and causes it to increase over time as well. The primary cause of inhomogeneity in the electrical properties is identified as energetic particle bombardment. Inhomogeneity in oxygen content is also observed, but its effect on the electrical properties is small and limited to the carrier mobility.

General information
State: Published
Organisations: Department of Micro- and Nanotechnology, Silicon Microtechnology, Department of Energy Conversion and Storage, Fundamental Electrochemistry, Department of Photonics Engineering, Optical Microsensors and Micromaterials, Department of Physics, Experimental Surface and Nanomaterials Physics, Technical University of Denmark
Authors: Crovetto, A. (Intern), Ottsen, T. S. (Ekstern), Stamate, E. (Intern), Kjær, D. (Intern), Schou, J. (Intern), Hansen, O. (Intern)
Number of pages: 11
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Volume: 49
Issue number: 29
Article number: 295101
ISSN (Print): 0022-3727
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 2.38 SJR 0.717 SNIP 1.011
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.07 SJR 1.135 SNIP 1.122
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.886 SNIP 1.25 CiteScore 2.1
On the Challenges of Reducing Contact Resistances in Thermoelectric Generators Based on Half-Heusler Alloys

A method using fast hot pressing to join half-Heusler (HH) thermoelectric materials directly to an electrical current collector (Ag electrode) without using a third filler material is introduced. The compositions of the HH alloys used are Hf0.5Zr0.5CoSn0.2Sb0.8 and Ti0.6Hf0.4NiSn for p- and n-type, respectively. Using this method, the quality of the...
HH–electrode contacts is improved due to their low electrical contact resistance and less reaction–diffusion layer. The microstructure and chemical composition of the joints were examined using a scanning electron microscope equipped with energy-dispersive x-ray analysis. The electrical characteristics of the interfaces at the contacts were studied based on electrical contact resistance and Seebeck scanning microprobe measurements. In this paper, we show that joining the HH to a Ag electrode directly using fast hot pressing resulted in lower contact resistance and better performance compared with the method of using active brazing filler alloy.
On the chemical synthesis route to bulk-scale skutterudite materials

In this article an alternative high yield route for the synthesis of CoSb$_3$-based unfilled skutterudites is presented. Using low-melting temperature salts of the constituents, melting and mixing them homogeneously in a hydrophobic liquid with postprocessing of the powders we achieve a more intimately mixed alloy compared to the conventional melting and metallurgical processes. The proposed method consists of a fast and low-temperature processing step followed by a thermochemical post-processing step, compared to the conventional methods of fabricating skutterudites, which require high temperatures and long processing times. Several structural characterization techniques were used to assess the mechanism of synthesis, verify the purity of the material as well as the reproducibility of the process. Detailed analysis and results are presented in support of the proposed process. Additionally, compaction of the powders with SPS technique provided a safe route to maintaining the nanopowder size and achieving low thermal conductivity (3 W/mK). The proposed method can easily be scaled up and adopted by the industry.

General information

State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, KTH - Royal Institute of Technology
Authors: Tafti, M. Y. (Ekstern), Saleemi, M. (Ekstern), Han, L. (Intern), Van Nong, N. (Intern), Toprak, M. S. (Ekstern)
Number of pages: 7
Pages: 5312-5318
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information

Journal: Ceramics International
Volume: 42
Issue number: 4
ISSN (Print): 0272-8842
Ratings:
- BFI (2018): BFI-level 1
- Web of Science (2018): Indexed yes
- BFI (2017): BFI-level 1
- Scopus rating (2017): CiteScore 2.85 SJR 0.784 SNIP 1.167
- Web of Science (2017): Indexed yes
- BFI (2016): BFI-level 1
- Scopus rating (2016): CiteScore 2.88 SJR 0.844 SNIP 1.376
- Web of Science (2016): Indexed yes
- BFI (2015): BFI-level 1
- Scopus rating (2015): SJR 0.823 SNIP 1.281 CiteScore 2.64
- Web of Science (2015): Indexed yes
- BFI (2014): BFI-level 1
- Scopus rating (2014): SJR 0.856 SNIP 1.645 CiteScore 2.76
- Web of Science (2014): Indexed yes
- BFI (2013): BFI-level 1
Operational stability of large scale OPV modules: interfaces, materials selection and stack design

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Functional organic materials
Authors: Roth, B. (Intern), Krebs, F. C. (Intern), Søndergaard, R. R. (Intern)
Number of pages: 135
Publication date: 2016

Publication information
Place of publication: Roskilde, Denmark
Publisher: Department of Energy Conversion and Storage, Technical University of Denmark
ISBN (Electronic): 978-87-92986-49-8
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
PhD_thesis_Berenger_Roth_print_red.pdf

Relations
Projects:
Operational stability of large scale OPV modules: interfaces, materials selection and stack design
We present a semi-analytical algorithm for magnet design problems, which calculates the optimal way to subdivide a given design region into uniformly magnetized segments. The availability of powerful rare-earth magnetic materials such as Nd-Fe-B has broadened the range of applications of permanent magnets[1][2]. However, the powerful rare-earth magnets are generally expensive, so both the scientific and industrial communities have devoted a lot of effort into developing suitable design methods. Even so, many magnet optimization algorithms either are based on heuristic approaches[3], or are applicable only to analytically solvable geometries[4]. In addition, some questions remained fundamentally unanswered, such as how to segment a given design into N uniformly magnetized pieces. Our method calculates the globally optimal shape and magnetization direction of each segment inside a certain design area with an optional constraint on the total amount of magnetic material. The method can be applied to any objective functional which is linear respect to the field, and with any combination of linear materials. Being based on an analytical-optimization approach, the algorithm is not computationally intensive and provides the global optimum with respect to the considered problem without the need for a starting guess. The approach can be used in combination with finite element method calculations, and can therefore be applied also to problems for which an analytical solution to the magnetic field is not available. We will illustrate the results for magnet design problems from different areas, such as electric motors/generators (as the example in the picture), beam focusing for particle accelerators and magnetic refrigeration devices.

We present an optimization approach which can be employed to calculate the globally optimal segmentation of a two-dimensional magnetic system into uniformly magnetized pieces. For each segment the algorithm calculates the optimal shape and the optimal direction of the remanent flux density vector, with respect to a linear objective functional. We illustrate the approach with results for magnet design problems from different areas, such as a permanent magnet electric motor, a beam focusing quadrupole magnet for particle accelerators and a rotary device for magnetic refrigeration.
The aim of this thesis is to investigate a framework to design and optimise magnetostatic systems. Over the course of the last decades the range of applications of permanent magnets expanded considerably, thanks to the development of powerful rare-earth permanent magnets. Concurrently, the research on methods to optimise permanent magnet based magnetic systems...
intensified. The increase in computational power, and the emergence of new optimisation algorithms provided new
instruments for the design of magnetic systems. All these factors contribute in making the optimisation of magnetic systems
a very lively sector of modern research.

The main focus of this work are magnetic systems based on permanent magnets, although hybrid systems combining
permanent magnets with electromagnets are also considered. Many optimisation approaches presented here are derived
within a framework based on the reciprocity theorem. This theorem formulates an energy equivalence principle with
several implications concerning the optimisation of objective functionals that are linear with respect to the magnetic field.
Linear functionals represent different optimisation goals, e.g. maximising a certain component of the field averaged over a
region of space. In general, a linear functional can be expressed as the integral over a given region of the scalar product
between the magnetic field and an arbitrarily defined objective vector field. It has been known for some time that the
reciprocity theorem can be used to determine the optimal remanence distribution with respect to a linear objective
functional.

Additionally, it is shown here that the same formalism can be applied to the optimisation of the geometry of magnetic
systems. Specifically, the border separating the permanent magnet from regions occupied by air or soft magnetic material
can be optimised within this framework. Since in the practice most structures are realized by assembling uniformly
magnetized pieces of permanent magnet, it is relevant to address the question of how a given region of space is best
subdivided. This problem is investigated here within the framework of the reciprocity theorem. Analytical derivations will be
used to show that, for segmentations controlled by a single parameter, the globally optimal solution to this problem can be
determined for almost arbitrary geometries. The case of segmentations depending by two parameters has been
approached employing a heuristic algorithm, which led to new design concepts. Some of the procedures developed for
linear objective functionals have been extended to non-linear objectives, by employing iterative techniques.

Even though most the optimality results discussed in this work have been derived analytically, the different approaches
have been implemented in combination with finite element methods, resulting in
flexible and computationally efficient algorithms. Most of the optimisation approaches could only be proven under the
assumption of linear magnetic behavior. The last part of this thesis also investigates some of the effects on the
performance of magnetic systems, due to non-linear magnetic phenomena. In particular, the non-linear demagnetization
effects caused by the finite coercivity of the permanent magnet material will be examined.

All the optimisation techniques will be illustrated with example magnetic systems for different applications, thus showing
the versatility and efficacy of the various approaches. The Halbach cylinder geometry, relevant for many applications, will
be often used as example, also because of the many symmetries and optimality properties exhibited by this geometry.
Despite the fact that this system has already been subject of many publications, some of the aspects considered in this
thesis have not been investigated before. The ultimate goal of the PhD project is to apply the optimisation techniques
developed during this research to the design of the magnetic system for the prototype of heat pump based on the
magnetocaloric effect. Magnetic systems for room temperature magnetic refrigeration will thus frequently be used as
illustrative examples along the course of this thesis.

Primarily because of the theoretical relevance of linear functionals, the results presented here lead to a deeper
understanding of the magnet optimisation process. One of the perspectives considered in this work is the trade-off
between field intensity and field quality, as the choice of a particular optimisation approach may favour one or the other.
The general framework discussed here provides a set of useful tools aiding the magnet design process. This research
also opened new scientific questions which would be worth investigating in future studies.

---

**Optimization of Catalyst Layer Properties for High Temperature Polymer Fuel Cells**

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors, Danish Power Systems ApS
Optimization of Multi-layer Active Magnetic Regenerator towards Compact and Efficient Refrigeration

Magnetic refrigerators can theoretically be more efficient than current vapor compression systems and use no vapor refrigerants with global warming potential. The core component, the active magnetic regenerator (AMR) operates based on the magnetocaloric effect of magnetic materials and the heat regeneration processes of periodic fluid blows. Magnetocaloric materials with a first order phase transition (FOPT) are suitable to realize a higher cooling capacity than commonly used gadolinium, but layering such materials is necessary, due to a large isothermal entropy change (ΔSiso) in a narrow region around their Curie temperature. Simulations are implemented to investigate how to layer the FOPT materials for obtaining higher cooling capacity. Moreover, based on entropy generation minimization, optimization of the regenerator geometry and related operating parameters is presented for improving the AMR efficiency. In addition, simulations are carried out to investigate the potential of applying nanofluid in future magnetic refrigerators.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, University of Southern Denmark
Publication date: 2016

Host publication information
Title of host publication: Proceedings of the 29th International Conference on Efficiency, Cost, Optimisation, Simulation and Environmental Impact of Energy Systems (ECOS 2016)
Article number: PAP-433
Main Research Area: Technical/natural sciences
Conference: 29th International Conference on Efficiency, Cost, Optimisation, Simulation and Environmental Impact of Energy Systems, Portorož, Slovenia, 19/06/2016 - 19/06/2016
Electronic versions:
Optimization_of_Multi_layer_Active.pdf

Bibliographical note
Presentation section: Refrigeration & air conditioning; Heat pumps
Source: PublicationPreSubmission
Source-ID: 127761814
Publication: Research - peer-review › Article in proceedings – Annual report year: 2016

Optimization of the Public Buildings Energy Supply: the case of the school in Koprivnica

There is a rising interest in the improvement of energy efficiency in public buildings nowadays at the EU level. Increasing energy efficiency can lead to both better thermal comfort, as well as net savings on energy bills. Furthermore, the right choice of energy source can lead to large savings in CO2 emissions. Recently, there have been a lot of projects in Croatia concerning the renovation of schools. However, many of them do not take the holistic approach during the refurbishment projects. They rather focus on a partial solution, focusing only on heating or heating and power supply. Furthermore, the choice of heating furnaces is often based on old and inaccurate data, without any mid or long term planning. In order to solve this issue, a simple to use continuous linear optimization model has been developed, which calculates the best investment options for heating, cooling and power supply. The model has a variety of choices and chooses the optimal one based on the external conditions entered, such as hourly temperatures, wind speed and global insolation. The model uses hourly time steps during one year, while the objective function of the developed model is to maximize net present
value of the project. The model was validated on a case of Antun Nemčić Gostovinski primary school in Koprivnica, Croatia. The school has 728 pupils and 77 employees and is open from 08 AM to 08 PM every working day. It also has two adjacent gyms, kitchen and the library. The model showed that significant savings could be achieved by taking a holistic approach during the refurbishment of the building, at the same time increasing thermal comfort of the students and employees. Finally, the developed model would be easy to adapt to any other similar public building, which could lead to further savings in energy consumption.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, University of Zagreb, Adria Section of the Combustion Institute
Authors: Filipović, P. (Ekstern), Dominkovic, D. F. (Intern), Ćosić, B. (Ekstern)
Pages: 160-160
Publication date: 2016

Host publication information
Title of host publication: Book of Abstracts : 11th Conference on Sustainable Development of Energy, Water and Environment Systems
Article number: SDEWES.SEE2016.0184
Main Research Area: Technical/natural sciences
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2016

Outdoor fate and environmental impact of polymer solar cells through leaching and emission to rainwater and soil
The emission of silver and zinc to the aqueous environment (rain, fog, dew) from polymer solar cells installed outdoors is presented. Studies included pristine solar cells and solar cells subjected to mechanical damage under natural weather conditions in Denmark. We find the emission of silver and zinc to the environment through precipitated water for damaged solar cells, and also observed failure and emission from an initially undamaged device in an experiment that endured for 6 months. In the case of the damaged cells, we found that the drinking water limits for Ag were only exceeded on a few single days. We also progressed our studies to include end-of-life management. To assess the implications of improper practices (uncontrolled disposal, landfilling) at the end-of-life, we buried different OPV types in intact and damaged forms in soil columns. In the case of high Ag emission (shredded cells), the potential for migration was confirmed, even though the soil was found to exhibit sequestration of silver. We conclude that recycling of Ag at the end-of-life is mandatory from an environmental point of view.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Functional organic materials, University of Applied Sciences and Arts Northwestern Switzerland
Authors: Espinosa Martinez, N. (Intern), Zimmermann, Y. (Ekstern), Benatto, G. A. D. R. (Intern), Lenz, M. (Ekstern), Krebs, F. C. (Intern)
Number of pages: 7
Published date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Energy & Environmental Science
Volume: 9
Number: 5
ISSN (Print): 1754-5692
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): SNIP 4.819 SJR 14.59 CiteScore 30.87
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 26.39 SJR 12.283 SNIP 4.325
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Oxygen permeation flux through 10Sc1YSZ-MnCo2O4 asymmetric membranes prepared by two-step sintering

Asymmetric membranes based on a dual phase composite consisting of (Y2O3)0.99(Sc2O3)0.1(ZrO2)0.89 (10Sc1YSZ) as ionic conductor and MnCo2O4 as electronic conductor were prepared and characterized with respect to sinterability, microstructure and oxygen transport properties. The composite membranes were prepared by tape casting, lamination and fired in a two-step sintering process. Microstructural analysis showed that a gastight thin membrane layer with the desired ratio of ionic/electronic conducting phases could be fabricated. Oxygen permeation fluxes across the 10ScdYSZ/MnCo2O4 (70/30 vol%) composite membrane were measured from 750 to 940 degrees C using air or pure oxygen as feed gases and N2 or CO2 as sweep gases. Fluxes up to 2.3 mlN min-1 cm-2 were obtained for the 7 μm thick membrane. A degradation test over 7730 h showed an initial degradation of 21% during the first 1100 h after which stable performance was achieved. The observed degradation is attributed to coarsening of the infiltrated catalyst. (C) 2016 Elsevier B.V. All rights reserved.
Oxygen Reduction Reaction on Pt Overlayers Deposited onto a Gold Film: Ligand, Strain, and Ensemble Effect

We study the oxygen reduction reaction (ORR), the catalytic process occurring at the cathode in fuel cells, on Pt layers prepared by electrodeposition onto an Au substrate. Using a nominal Pt layer by layer deposition method previously proposed, imperfect layers of Pt on Au are obtained. The ORR on deposited Pt layers decreases with increasing Pt thickness. In the submonolayer region, however, the ORR activity is superior to that of bulk Pt. Using density functional theory (DFT) calculations, we correlate the observed activity trend to strain, ligand, and ensemble effects. At submonolayer coverage certain atom configurations weaken the binding energies of reaction intermediates due to a ligand and ensemble effect, thus effectively increasing the ORR activity. At higher Pt coverage the activity is governed by a strain effect, which lowers the activity by decreasing the oxidation potential of water. This study is a nice example of how the influence of strain, ligand, and ensemble effects on the ORR can be deconvoluted.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, University of Copenhagen
Authors: Deng, Y. (Ekstern), Tripkovic, V. (Intern), Rossmeisl, J. (Ekstern), Arenz, M. (Ekstern)
Number of pages: 6
Pages: 671-676
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: A C S Catalysis
Volume: 6
Issue number: 2
ISSN (Print): 2155-5435
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 11.49 SJR 4.921 SNIP 2.113
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 10.3 SJR 4.367 SNIP 2.081
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 3.973 SNIP 2.119 CiteScore 9.88
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 3.67 SNIP 2.02 CiteScore 8.74
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 3.301 SNIP 1.848 CiteScore 7.41
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Scopus rating (2012): SJR 2.729 SNIP 1.619 CiteScore 5.19
ISI indexed (2012): ISI indexed no
Web of Science (2012): Indexed yes
ISI indexed (2011): ISI indexed no
Original language: English
Oxygen reduction reaction, Pt, Au, Ligand effect, Strain effect, Ensemble effect
Electronic versions:
Deng_et_al._The_oxygen_reduction_reaction_on_Pt_overlayers_deposited_onto_a_gold_film_ligand_strain_and.pdf.
Embargo ended: 08/12/2017
DOIs:
10.1021/acscatal.5b02409
Source: FindIt
Source-ID: 2289638111
Publication: Research - peer-review › Journal article – Annual report year: 2016
Patterning and Conductivity Modulation of Conductive Polymers by UV Light Exposure

A novel patterning technique of conductive polymers produced by vapor phase polymerization is demonstrated. The method involves exposing an oxidant film to UV light which changes the local chemical environment of the oxidant and subsequently the polymerization kinetics. This procedure is used to control the conductivity in the conjugated polymer poly(3,4-ethylenedioxythiophene):tosylate by more than six orders of magnitude in addition to producing high-resolution patterns and optical gradients. The mechanism behind the modulation in the polymerization kinetics by UV light irradiation as well as the properties of the resulting polymer are investigated.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Imaging and Structural Analysis, Linköping University, University of South Australia
Number of pages: 11
Pages: 6950-6960
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Advanced Functional Materials
Volume: 26
Issue number: 38
ISSN (Print): 1616-301X
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 12.51
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 11.56
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 11.93
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 11.32
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 10.6
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 10.41
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 9.47
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 2
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Web of Science (2008): Indexed yes
Web of Science (2007): Indexed yes
Performance and Lifetime Limiting Effects in Li-ion Batteries

Lithium-ion batteries (LIBs) find widespread use for electricity storage, from portable devices such as smart phones to electric vehicles (EV), because of their high energy density and design flexibility. However, limited lifetime is still a challenge for several LIB materials. Specifically, the detailed coupling between degradation mechanisms and battery usage is not fully understood, which impedes lifetime improvements. To understand the degradation mechanisms and increase the performance of these materials, the development of improved characterization methods is crucial. This PhD thesis focuses on the thorough analysis of degradation mechanism in LIBs, trying to relate morphological and structural changes in Lithium-ion battery electrodes to performance degradation observed during electrode cycling. Degradation mechanisms in laboratory scale LFP cathodes were correlated with the degradation mechanisms observed in commercial LIBs. The structural and morphological changes in cycled laboratory LFP cathodes were studied by low-kV FIB/SEM Tomography and TEM analysis and related to the electrode performance using Electrochemical Impedance Spectroscopy (EIS). The two main degradation processes observed by microscopy analysis in the aged electrode were cracking of LFP particles and agglomeration of carbon black (CB) additive. The increased heterogeneity of the CB network reduces the electron percolation throughout the porous electrode, thereby decreasing the amount of electrochemically active LFP particles. The electron resistivity was quantified with the EIS analysis using a Transmission Line Model (TLM) developed for porous LFP electrodes. Similar TLM models were applied for the analysis of the polarization processes in a commercial LFP and graphite electrodes. The microscopy analysis of the electrodes showed the presence of carbonaceous agglomerates on the electrode/electrolyte interfaces. The agglomerates are expected to increase the ionic resistance and be related to loss of lithium inventory (LLI).
the electrochemical three-phase-boundary reaction zone in the presence of GDC must be very limited and cannot account for the higher sulfur tolerance of GDC modified SOFC anodes.

**General information**

State: Published  
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry, Ceramic Engineering & Science, Mixed Conductors  
Authors: Nielsen, J. (Intern), Sudireddy, B. R. (Intern), Hagen, A. (Intern), Persson, Å. H. (Intern)  
Publication date: 2016  
Main Research Area: Technical/natural sciences

**Publication information**

Journal: Journal of the Electrochemical Society  
Volume: 163  
Issue number: 6  
ISSN (Print): 0013-4651  
Ratings:  
BFI (2018): BFI-level 1  
Web of Science (2018): Indexed yes  
BFI (2017): BFI-level 1  
Scopus rating (2017): CiteScore 3.48 SJR 1.267 SNIP 1.009  
Web of Science (2017): Indexed yes  
BFI (2016): BFI-level 1  
Scopus rating (2016): CiteScore 2.97 SJR 1.222 SNIP 0.963  
Web of Science (2016): Indexed yes  
BFI (2015): BFI-level 1  
Scopus rating (2015): SJR 1.115 SNIP 1.066 CiteScore 3.17  
Web of Science (2015): Indexed yes  
BFI (2014): BFI-level 1  
Scopus rating (2014): SJR 1.213 SNIP 1.25 CiteScore 3.36  
Web of Science (2014): Indexed yes  
BFI (2013): BFI-level 1  
Scopus rating (2013): SJR 1.169 SNIP 1.309 CiteScore 2.92  
ISI indexed (2013): ISI indexed yes  
Web of Science (2013): Indexed yes  
BFI (2012): BFI-level 1  
Scopus rating (2012): SJR 1.329 SNIP 1.281 CiteScore 2.61  
ISI indexed (2012): ISI indexed yes  
Web of Science (2012): Indexed yes  
BFI (2011): BFI-level 1  
Scopus rating (2011): SJR 1.331 SNIP 1.335 CiteScore 2.74  
ISI indexed (2011): ISI indexed yes  
Web of Science (2011): Indexed yes  
BFI (2010): BFI-level 1  
Scopus rating (2010): SJR 1.418 SNIP 1.304  
Web of Science (2010): Indexed yes  
BFI (2009): BFI-level 1  
Scopus rating (2009): SJR 1.442 SNIP 1.27  
Web of Science (2009): Indexed yes  
BFI (2008): BFI-level 1  
Scopus rating (2008): SJR 1.595 SNIP 1.41  
Web of Science (2008): Indexed yes  
Scopus rating (2007): SJR 1.569 SNIP 1.322  
Web of Science (2007): Indexed yes  
Scopus rating (2006): SJR 1.608 SNIP 1.535  
Web of Science (2006): Indexed yes
Performance of Halbach magnet arrays with finite coercivity

A numerical method to study the effect of finite coercivity on the Halbach cylinder geometry is presented. Despite the fact that the analytical solution available for this geometry does not set any limit to the maximum air gap flux density achievable, in real life the non-linear response of the magnetic material and the fact that the coercivity is not infinite will limit the attainable field. The presented method is able to predict where and when demagnetization will occur, and these predictions are compared with the analytical solution for the case of infinite coercivity. However, the approach presented here also allows quantification of the decrease in flux density and homogeneity for a partially demagnetized magnet. Moreover, the problem of how to realize a Halbach cylinder geometry using a mix of materials with different coercivities without altering the overall performance is addressed. Being based on a numerical approach, the presented method can be employed to analyze the demagnetization effects due to coercivity for any geometry, even when the analytical solution is not available.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Authors: Insinga, A. R. (Intern), Bahl, C. (Intern), Bjørk, R. (Intern), Smith, A. (Intern)
Number of pages: 8
Pages: 369-376
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Magnetism and Magnetic Materials
Volume: 407
ISSN (Print): 0304-8853
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SJR 0.786 SNIP 1.349 CiteScore 2.97
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.41 SJR 0.699 SNIP 1.181
Web of Science (2016): Indexed yes

Performance of Halbach magnet arrays with finite coercivity

A numerical method to study the effect of finite coercivity on the Halbach cylinder geometry is presented. Despite the fact that the analytical solution available for this geometry does not set any limit to the maximum air gap flux density achievable, in real life the non-linear response of the magnetic material and the fact that the coercivity is not infinite will limit the attainable field. The presented method is able to predict when and where demagnetization will occur, and these predictions are compared with the analytical solution for the case of infinite coercivity. However, the approach presented here also allows quantification of the decrease in flux density and homogeneity for a partially demagnetized magnet. Moreover, the problem of how to realize a Halbach cylinder geometry using a mix of materials with different coercivities without altering the overall performance is addressed. Being based on a numerical approach, the presented method can be employed to analyze the demagnetization effects due to coercivity for any geometry, even when the analytical solution is not available.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Authors: Insinga, A. R. (Intern), Bahl, C. (Intern), Bjørk, R. (Intern), Smith, A. (Intern)
Number of pages: 8
Pages: 369-376
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Magnetism and Magnetic Materials
Volume: 407
ISSN (Print): 0304-8853
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SJR 0.786 SNIP 1.349 CiteScore 2.97
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.41 SJR 0.699 SNIP 1.181
Web of Science (2016): Indexed yes
Due to the attractive properties of nanoparticles because of their effective surface area, they have been studied widely. Nano-yttria-stabilized zirconia (n-YSZ) is a ceramic which has been scrutinized extensively in past years. Because of the...
different stability behavior of n-YSZ in comparison with bulk YSZ, a new phase diagram is needed for the n-YSZ system in order to identify stable phases under various conditions. In this study, a phase diagram for the n-YSZ system was provided to determine phase stability ranges at room temperature with respect to particle size and composition. The calculation of phase diagrams (CALPHAD) approach was applied to calculate the Gibbs energy of bulk YSZ. It was combined with the surface energy of each phase in the n-YSZ system, i.e. monoclinic, tetragonal, cubic, and amorphous, to produce the total Gibbs energy of each individual phase of the n-YSZ system. By applying the CALPHAD approach, a 3-D phase diagram for the n-YSZ system was established in which the stability range of each individual phase can be predicted based on the particle size, composition, and temperature.

Plasma diagnostics during magnetron sputtering of aluminum doped zinc oxide

Plasma parameters during magnetron sputtering of aluminum-doped zinc oxide are investigated with optical emission spectroscopy, electrostatic probes and mass spectrometry with the aim of understanding the role of negative ions of oxygen during the film growth and improving the uniformity of the film resistivity over the deposition area.
Platinum Iron Intermetallic Nanoparticles Supported on Carbon Formed In Situ by High-Pressure Pyrolysis for Efficient Oxygen Reduction

Carbon-supported PtFe alloy catalysts are synthesized by the one-step, high-temperature pyrolysis of Pt, Fe, and C precursors. As a result of the high temperature, the formed PtFe nanoparticles possess highly ordered, face-centered tetragonal, intermetallic structures with a mean size of ≈11.8 nm. At 0.9 V versus the reversible hydrogen electrode, the PtFe nanoparticles show a 6.8 times higher specific activity than the reference Pt/C catalyst towards the oxygen reduction reaction (ORR) as well as excellent stability, most likely because of the durable intermetallic structure and the preleaching treatment of the catalyst. During these preliminary syntheses, we found that a portion of the PtFe nanoparticles is buried in the in situ formed carbon phase, which limits Pt utilization in the catalyst and results in a mass-specific activity equivalent to the commercial Pt/C catalyst. Moreover, the possible presence of other active sites, for example, FeNₓ, CNₓ, and carbon-encapsulated metal nanoparticles, and their contribution to the ORR performance of the catalyst are also investigated.
Playing with Light in Organic Thin-Film Solar Cells

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Organic Energy Materials
Authors: Pastorelli, F. (Intern)
Number of pages: 1
Publication date: 2016
Event: Abstract from 2016 MRS Fall Meeting & Exhibit, Boston, MA, United States.
Main Research Area: Technical/natural sciences
Electronic versions:
Playing_with_Light.pdf

Bibliographical note
Symposium NM4 : Nanomaterials-Based Solar Energy Conversion
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2016

Play with light in thin film organic materials: from nanoscale to smart windows

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Organic Energy Materials
Authors: Pastorelli, F. (Intern)
Publication date: 2016

Publication information
Media of output: Video
Original language: English
Publisher: DTU Energy
Main Research Area: Technical/natural sciences
Links:
https://youtu.be/tb_Dq-OMPnQ

Bibliographical note
Invited talk
Source: PublicationPreSubmission
Source-ID: 127807154
Publication: Research - peer-review › Sound/Visual production (digital) – Annual report year: 2016
Polaronic motion of self-trapped holes in silver halides

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, Universidad de Cantabria
Authors: García Lastra, J. M. (Intern), Garcia-Fernandez, P. (Ekstern), Loftager, S. (Intern), Aramburu, J. (Ekstern), Moreno, M. (Ekstern)
Number of pages: 1
Publication date: 2016
Event: Abstract from International Conference on Defects in Insulating Materials (ICDIM 2016), Lyon, France.
Main Research Area: Technical/natural sciences
Electronic versions:
Polaronic_motion.pdf
Source: PublicationPreSubmission
Source-ID: 128083480
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2016

Polybenzimidazole Membranes by Post Acid Doping

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors
Authors: Aili, D. (Intern), Jensen, J. O. (Intern), Li, Q. (Intern)
Pages: 195-215
Publication date: 2016

Host publication information
Title of host publication: High Temperature Polymer Electrolyte Membrane Fuel Cells: Approaches, Status, and Perspectives
Place of publication: Switzerland
Publisher: Springer
Editors: Li, Q., Aili, D., Hjuler, H. A., Jensen, J. O.
ISBN (Print): 978-3-319-17081-7
ISBN (Electronic): 978-3-319-17082-4
Chapter: 9
Main Research Area: Technical/natural sciences
DOIs:
10.1007/978-3-319-17082-4_9
Publication: Research - peer-review › Book chapter – Annual report year: 2016

Polybenzimidazole membranes for zero gap alkaline electrolysis cells
Membranes of m-PBI doped in KOH (aq), 15-35 wt%, show high ionic conductivity in the temperature range 20-80 °C. In electrolysis cells with nickel foam electrodes m-PBI membranes provide low internal resistance. With a 60 µm membrane at 80°C in 20 wt% KOH, 1000 mA/cm² is achieved at 2.25.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors
Authors: Kraglund, M. R. (Intern), Aili, D. (Intern), Christensen, E. (Intern), Jensen, J. O. (Intern)
Number of pages: 1
Publication date: 2016
Event: Poster session presented at The 21st World Hydrogen Energy Conference (WHEC), Zaragoza, Spain.
Main Research Area: Technical/natural sciences
Electronic versions:
WHEC2016_polbenzimidazole_membranes_for_zero_gap_alkaline_electrolysis_cells.pdf
Source: PublicationPreSubmission
Source-ID: 125388571
Publication: Research - peer-review › Poster – Annual report year: 2016

Polymer materials for roll coated solar cells: strategies to improve performance and stability
Solar cells are among the renewable energy technologies with a large potential in terms of solar energy availability. The solar cells based on conjugated polymers belong to the third generation of this technology and their attractive features
include a fast and cheap solution-processed production. At DTU Energy the focus is the roll-to-roll coating process of these materials in order to reach large area devices, as the processability and scalability of the technology is an important factor. The process ability using roll-coating techniques and the stability of the used materials can be crucial. Therefore this project focuses on the synthesis of conjugated polymers and their application in roll-coated polymer solar cells. The first part of this project aims at using a screening strategy to find suitable polymer candidates for well performing solution processed polymer solar cells. A large number of polymers was screened by applying them in roll-coated solar cells and their performance, stability and number of synthetic steps was compared, to find promising candidates. In the end seven polymers with a sufficient efficiency were found to behave in a higher or in similar manner as poly(3-hexylthiophene). Further polymers were prepared based on well performing benzothiadiazole and thiophene based polymers with different incorporation ratios of these monomers. The incorporation ratio has different effects on the polymer properties and the performance and stability of the corresponding roll-coated devices. The best efficiency was achieved with a polymer by using an incorporation of four thiophenes in the repeating unit. The second part of the work aims at using a known strategy to improve the solar cells stability. Three of the polymers from the polymer screening were therefore partly modified with stabilizing side chains, 2-phenetyl and 2-ethanol, respectively, to influence especially the device stability but also the performance. For most modifications a decrease of the solar cell efficiency was observed. The incorporation of 10% of these side chains show improvements of the stability of devices in a minor degree with a variation in the photo- and thermal stability. In addition to the use of different side chains, the impact of different positioning of one side chain was investigated, showing that the incorporation onto the acceptor or donorunit of the polymer showed a degradation or improvement of the resulting properties. In addition, the approach of side chain removable on polythiophene was compared in terms of optical properties and morphologies of two polymers with different (thermal or acidic) cleavage processes. It was found that their properties were not the same and therefore different results from the corresponding solar cells can be expected.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Organic Energy Materials
Authors: Heckler, I. M. (Intern), Bundgaard, E. (Intern)
Number of pages: 234
Publication date: 2016

Publication information
Place of publication: Kgs. Lyngby
Publisher: Department of Energy Conversion and Storage, Technical University of Denmark
ISBN (Print): 978-87-92986-59-7
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
Ilona_Heckler_PhD_thesis_DTU_Energy.pdf

Relations
Projects:
Polymer materials for roll coated solar cells: strategies to improve performance and stability
Publication: Research › Ph.D. thesis – Annual report year: 2017

Poly(vinylpyrrolidone) as dispersing agent for cerium-gadolinium oxide (CGO) suspensions
The behaviour of selected poly(vinylpyrrolidone) grades to act as dispersant for ethanol-based cerium gadolinium oxide suspensions was investigated and related to the molecular weight characteristics. The number, weight, and z-average molecular weights \( M_n \), \( M_w \), and \( M_z \) were determined by gel permeation chromatography and then used in a numerical method to evaluate the viscosity average molecular weight (\( M_v \)) via an empirically modified Mark–Houwink–Sakurada (MHS) equation. The MHS equation parameters (\( a \) and \( K \)) and the polydispersity correction factor (\( q_{MHS} \)) were also evaluated. Three grades with different molecular weight features were selected and further studied as dispersants by means of rheology. Despite the differences, only slight shifts in the amount of polymer required for achieving fully stabilized dispersions were observed, whereas comparable packing properties were obtained. This was explained as an effect of the polydispersity, expressed as \( q_{MHS} \).

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Department of Micro- and Nanotechnology, Center for Nanostructured Graphene, Self-Organized Nanoporous Materials, Mixed Conductors
Authors: Marani, D. (Intern), Sudireddy, B. R. (Intern), Nielsen, L. (Intern), Ndoni, S. (Intern), Kiebach, W. (Intern)
Pages: 1098-1106
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Portable and wireless IV-curve tracer for >5 kV organic photovoltaic modules

The practical design of a wirelessly controlled portable IV-curve tracer based on a capacitive load is described. The design is optimized for the measurement of solar cell modules presenting a high open circuit voltage of up to 6 kV and a low short circuit current below 100 mA. The portable IV-tracer allows for on-site/in-situ characterization of large modules under real operating conditions and enables fast detection of potential failure of anomalies in electrical behavior. Currently available electronic loads only handle voltages up to around 1 kV. To overcome cost and safety issues related to high voltage applications, the design is based on low cost components, battery-based isolated supply and wireless communication. A prototype has been implemented and field tested for characterization of different organic photovoltaic modules (OPV) made according to the infinity concept with a large number of serially connected single junctions (~7,450 single junctions) presenting open circuit voltages up to 5.6 kV.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Functional organic materials, Technical University of Cartagena
Number of pages: 6
Pages: 60-65
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Solar Energy Materials and Solar Cells
Volume: 151
ISSN (Print): 0927-0248
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 4.83 SJR 1.459 SNIP 1.532
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.97 SJR 1.599 SNIP 1.71
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.8 SNIP 1.851 CiteScore 5.16
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.19 SNIP 2.348 CiteScore 5.87
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 2.179 SNIP 2.529 CiteScore 5.58
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.441 SNIP 2.654 CiteScore 5.25
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
A facile green recipe was developed to synthesise highly pure, safe and durable zinc oxide nanoparticles (ZnO Nps) using homemade starch-rich potato extract. The ZnO Nps were synthesised using zinc nitrate and potato extract, and the whole reaction is carried out for 30 min at 80 °C. In the synthesis, starch-rich potato extract acted as the reducing agent and as a stabilising layer on freshly formed ZnO Nps. Hexagonal (wurtzite) shaped ZnO Nps with size about 20 ± 1.2 nm were synthesised and characterised using X-ray diffraction, transition electron microscope and scanning microscopy analyses. Fourier transform infrared spectral analysis indicated that highly pure ZnO nanopowders were obtained at higher temperatures. The use of environmentally benign and renewable material as the respective reducing and protecting agents, starch-rich potato extract, as well as a gentle solvent medium (H2O), offered a simple and quite efficient procedure for the synthesis of ZnO Nps in neutral medium with promising potential for biological and biomedical applications.
Preparation and Characterization of Cathode Materials for Lithium-Oxygen Batteries

A possible future battery type is the Li-air battery which theoretically has the potential of reaching gravimetric energy densities close to those of gasoline. The Li-air battery is discharged by the reaction of Li-ions and oxygen, drawn from the air, reacting at the battery cathode to form Li$_2$O$_2$. The type of cathode material affects the battery discharge capacity and charging potential and with a carbon based cathode many questions are still unanswered. The focus of this Ph.D. project has been the synthesis of reduced graphene oxide as well as the investigation of the effect of reduced graphene oxide as a cathode material, combined with in situ investigations of the formation of decomposition products in and on the cathode. The reduced graphene oxide was synthesized by the modified Hummers method followed by thermal reduction of graphene oxide, while both were investigated by in situ X-ray diffraction. This study revealed an early formation of graphene oxide, new graphene oxide diffraction peaks and an unidentified crystal phase along with a disordered stage of thethermal reduction of graphene oxide. The oxidation time effect on graphene oxide, synthesized by the modified Hummers method, and the following chemically and thermal reduced graphene oxide was investigated. This revealed that trends introduced by changes in oxidation time were observed not only for the graphene oxide but also transcribed to both types of reduced graphene oxide. Furthermore the change in oxidation time affected the discharge capacity of the battery as well as the charging potential. In situ X-ray diffraction studies on carbon black cathodes in a capillary battery showed the formation of crystalline Li$_2$O$_2$ on the first discharge cycle, the intensity of Li$_2$O$_2$ on the second discharge cycle was however diminished. The study furthermore showed how X-rays may affect the Li$_2$O$_2$ battery, displaying how in situ studies may be invasive. An in situ X-ray diffraction study of a reduced graphene oxide cathode showed formation of both LiOH and Li$_2$O$_2$, which also was observed in cells with and without addition of water by XPS. The addition of water to the electrolyte gave indications of additional reactions taking place in the cell. The information provided in this study is useful for a better understanding of reduced graphene oxide both in regards to synthesis and as cathode material in Li-air batteries. The thesis illuminates the importance of considering the synthesis of reduced graphene oxide as this seems to be couple to the abilities as cathode materials in Li-air batteries. It furthermore introduces two types of capillary battery designs optimized for Li-air and in situ X-ray diffraction, but with possibilities within metal-air batteries in general, and it opens up for a discussion of how invasive in situ methods may be.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, Stanford University
Authors: Storm, M. M. (Intern), Norby, P. (Intern), Luntz, A. C. (Ekstern)
Number of pages: 179
Publication date: 2016
Preparation and characterization of MgB$_2$ with Pd, Pt and Re doping

Samples with Mg$_{1-x}$D$_x$B$_2.04$ (D = Pt, Pd or Re) nominal compositions have been synthesised by a solid-state route. None of these doping elements can be substituted for Mg in a detectable amount and their presence in the samples has no influence on the critical temperature and on the lattice parameters of the MgB$_2$ superconductor. Impurity phases are formed by reaction mostly with Mg. The microstructure of the Pt, Pd and Re-based phases depends on the elements. Re-rich particles with large sizes up to 8 μm form, whereas Pt- and Pd-containing impurities are finely dispersed with a particle size that does not exceed 1 μm. The field dependence of the normalised critical current density is improved when Pt, Pd or Re are present in the samples.
Preparation and characterization of Sc doped MgB$_2$ wires

The in-situ technique was used to manufacture scâldium (Sc) doped MgB$_2$ wires in a composite Cu–Nb sheath. After reaction at 700 °C, at most 1 at. % Mg was replaced by Sc in the MgB$_2$ phase, without significant influence on its superconducting transition temperature. For higher Sc concentrations in the nominal composition, the formation of Sc–rich impurity phases was evidenced by SEM/EDS observations. The critical current density and accommodation field of the wires are weakly dependant on the Sc content. It is believed that these effects are related more to modifications of the thermal behaviour of the precursor powders revealed by DTA measurements than to actual doping. The best performance was obtained in a wire with Mg:Sc = 0.995 ± 0.005 atomic ratio.

General information

State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Polytechnical University of Bucharest
Authors: Grivel, J. (Intern), Burdusel, M. (Ekstern)
Number of pages: 8
Pages: 65-72
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Physica C: Superconductivity and its Applications
Volume: 528
Preparation, structure study and electrochemistry of layered $\text{H}_2\text{V}_3\text{O}_8$ materials: High capacity lithium-ion battery cathode

The present study explores $\text{H}_2\text{V}_3\text{O}_8$ as high capacity cathode material for lithium-ion batteries (LIB's). Despite having high discharge capacity, $\text{H}_2\text{V}_3\text{O}_8$ material suffers from poor electrochemical stability for prolonged cycle life. Ultra-long $\text{H}_2\text{V}_3\text{O}_8$ nanobelts with ordered crystallographic patterns are synthesized via a hydrothermal process to mitigate this problem. The growth of the crystal is facile along [001] direction, and the most common surface is (001) as suggested by Wulff construction study. Electrochemical performance of $\text{H}_2\text{V}_3\text{O}_8$ cathode is tested against Li/Li$^+$ at various current rates. At 50 mA g$^{-1}$ current rate, it delivers a discharge capacity of 308 mAh g$^{-1}$, whereas, at 3000 mA g$^{-1}$, an initial discharge capacity of 144 mAh g$^{-1}$ is observed and stabilized at 100 mAh g$^{-1}$ till 500 cycles. Further, the density functional theory (DFT) based simulations study of both the pristine and lithiated phase of $\text{H}_2\text{V}_3\text{O}_8$ cathode materials is undertaken. DFT study reveals the presence of hydrogen as hydroxyl unit in the framework of the host. In correlation, the magnetic property of vanadium atoms is examined in detail with through partial density of states (PDOS) calculation during three stage lithiation processes and evaluating various potential steps involved in lithium insertion.

General information

State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, Center for Study of Science, Technology and Policy, Indian Institute of Technology, Bombay
Authors: Sarkar, S. (Ekstern), Bhowmik, A. (Intern), Pan, J. (Intern), Bharadwaj, M. D. (Ekstern), Mitra, S. (Ekstern)
Number of pages: 11
Pages: 179-189
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information

Journal: Journal of Power Sources
Volume: 329
ISSN (Print): 0378-7753
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 7 SJR 2.202 SNIP 1.536
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 6.22 SJR 1.944 SNIP 1.5
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.9 SNIP 1.667 CiteScore 6.34
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.964 SNIP 2.042 CiteScore 6.3
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.975 SNIP 2.137 CiteScore 5.63
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.282 SNIP 2.006 CiteScore 5.04
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.227 SNIP 2.172 CiteScore 5.13
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
Pressurized Operation of a Planar Solid Oxide Cell Stack

Solid oxide cells (SOCs) can be operated either as fuel cells (SOFC) to convert fuels to electricity or as electrolyzers (SOEC) to convert electricity to fuels such as hydrogen or methane. Pressurized operation of SOCs provide several benefits on both cell and system level. If successfully matured, pressurized SOEC based electrolyzers can become more efficient both energy- and cost-wise than PEM and Alkaline systems. Pressurization of SOFCs can significantly increase the cell power density and reduce the size of auxiliary components. In the present study, a SOC stack was successfully operated at pressures up to 25 bar. The pressure dependency of the measured current-voltage (I-V) curves and impedance spectra on the SOC stack are analyzed and the relation between various system parameters and pressure is derived. With increasing pressure the open circuit voltage (OCV) and the reaction kinetics (electrode performance) increases for thermodynamic and kinetic reasons, respectively. Further, the summit frequency of the gas concentration impedance arc and the pressure difference across the stack and heat exchangers is seen to decrease with increasing pressure following a power-law expression. Finally a durability test was conducted at 10 bar.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry, Mixed Conductors
Authors: Jensen, S. H. (Intern), Sun, X. (Intern), Ebbesen, S. D. (Intern), Chen, M. (Intern)
Number of pages: 14
Pages: 205–218
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Fuel Cells
Volume: 16
Issue number: 2
ISSN (Print): 1615-6846
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 1.88 SJR 0.559 SNIP 0.748
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.79 SJR 0.495 SNIP 0.603
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.685 SNIP 0.779 CiteScore 2.02
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.615 SNIP 0.792 CiteScore 2.05
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.835 SNIP 0.833 CiteScore 1.99
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.24 SNIP 0.993 CiteScore 2.76
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.639 SNIP 1.247 CiteScore 3.31
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.623 SNIP 1.236
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.36 SNIP 1.108
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.506 SNIP 1.211
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.338 SNIP 1.074
Scopus rating (2006): SJR 1.186 SNIP 1.209
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.449 SNIP 0.496
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.259 SNIP 0.348
Web of Science (2004): Indexed yes
Web of Science (2001): Indexed yes
Original language: English
Durability, Electrochemical Impedance Spectroscopy, I-V curves, Planar, Pressure, Solid Oxide Cell, Stack, Electrochemical impedance spectroscopy
Electronic versions: presurized.pdf. Embargo ended: 12/02/2017
DOIs: 10.1002/fuce.201500180
Source: FindIt
Source-ID: 2292082853
Publication: Research - peer-review › Journal article – Annual report year: 2016
Printable luminescent down shifter for enhancing efficiency and stability of organic photovoltaics

The proof of concept of using luminescent down shifting (LDS) layers as alternative UV filters for P3HT:PCBM OPVs is demonstrated using a lanthanide-based metal complex. The results are verified using a combination of indoor light soaking, with single cell devices, and outdoor performance monitoring, using a 16-cell monolithically connected OPV module. By applying the LDS layer, a ~5% relative enhancement in photocurrent is observed for both sets of devices. More significantly, indoor light soaking tests on single cell devices without encapsulation showed an 850% enhancement in the measured half-life (T50%). The OPV modules were encapsulated and tested for outdoor stability over a 70 day period in the Negev desert, Israel. The modules made with the LDS filter are shown to match the stability of those made with a commercial UV filter and outperform the modules with no filter applied, with a 51% enhancement in the measured stability (T75%). Significantly, the work provides clear experimental evidence that the LDS layer can act as a UV filter in OPVs without compromising the efficiency of the solar cell, thus providing an added benefit over commercial UV filters.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Functional organic materials, Bangor University, Ben-Gurion University of the Negev, Swansea University
Authors: Kettle, J. (Ekstern), Bristow, N. (Ekstern), Gethin, D. (Ekstern), Tehrani, Z. (Ekstern), Moudam, O. (Ekstern), Li, B. (Ekstern), Katz, E. (Ekstern), Benatto, G. A. D. R. (Intern), Krebs, F. C. (Intern)
Pages: 481–487
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Volume: 144
ISSN (Print): 0927-0248
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 4.83 SJR 1.459 SNIP 1.532
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.97 SJR 1.599 SNIP 1.71
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.8 SNIP 1.851 CiteScore 5.16
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.19 SNIP 2.348 CiteScore 5.87
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 2.179 SNIP 2.529 CiteScore 5.58
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.441 SNIP 2.654 CiteScore 5.25
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.182 SNIP 2.577 CiteScore 5.16
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 2.494 SNIP 2.105
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.942 SNIP 1.957
Probing the active site structures of iron-based ORR catalysts

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors
Authors: Hu, Y. (Intern), Li, Q. (Intern), Jensen, J. O. (Intern), Zhong, L. (Intern), Cleemann, L. N. (Intern)
Publication date: 2016
Conference: PRIME 2016/230th ECS Meeting, Honolulu, United States, 02/10/2016 - 02/10/2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Electrochemical Society. Meeting Abstracts (Online)
Volume: MA2016-02
Article number: 2771
ISSN (Print): 2151-2043
Original language: English
Links:
http://ma.ecsdl.org/content/MA2016-02/38/2771.abstract?sid=9220813d-2d81-4fd3-834c-3acb5da2f24f
Source: PublicationPreSubmission
Source-ID: 127806385
Publication: Research - peer-review › Conference abstract in journal – Annual report year: 2016

Processing and characterization of multilayers for energy device fabrication (invited)
The performance of asymmetric multilayer structures in solid oxide fuel cells (SOFC)/solid oxide electrolysis cells (SOEC), tubular oxygen transport membranes (OTM) and similar high temperature energy devices is often determined by the ceramic fabrication (for given materials and design). A good understanding and control of different processing steps (from powder/materials selection, through shaping and sintering) is of crucial importance to achieve a defect-free multilayer microstructure with the desired properties and performance.

Based on the experiences at DTU Energy with the fabrication of planar SOFC and tubular OTM, we present selected challenges in ceramic processing such asymmetric multilayer structures. By optimizing different steps in the ceramic processing, we improved the mechanical properties and gas permeability of porous supports and the (electrochemical) performance of electrodes/catalytic layers. Optical dilatometry has proven to be a powerful and fast tool to optimize the...
co-sintering of planar, asymmetric multilayers, consisting of a porous support and a dense membrane layer. The monitoring of dimensional changes and distortions in single and multilayers during de-binding and sintering allows the minimization of sintering stresses, thereby avoiding the formation of defects, such as camber, delamination or crack formation. We briefly highlight recent activities at DTU Energy with advanced processing techniques, such as using electrospinning and 3D printing in fabrication of multilayers.

**General information**

State: Published  
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Mixed Conductors  
Authors: Kaiser, A. (Intern), Kiebach, W. (Intern), Gurauskis, J. (Intern), Bjørnetun Haugen, A. (Intern), Ramousse, S. (Intern), Hendriksen, P. V. (Intern)  
Number of pages: 1  
Publication date: 2016  
Main Research Area: Technical/natural sciences  
Electronic versions:  
A_Kaiser_Abstract_DKG_Jahrestagung_2016_Freiberg.pdf  
Source: PublicationPreSubmission  
Source-ID: 141858253  
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2017

**Promising bulk nanostructured Cu2Se thermoelectrics via high throughput and rapid chemical synthesis**

A facile and high yield synthesis route was developed for the fabrication of bulk nanostructured copper selenide (Cu2Se) with high thermoelectric efficiency. Starting from readily available precursor materials and by means of rapid and energy-efficient microwave-assisted thermolysis, nanopowders of Cu2Se were synthesized. Powder samples and compacted pellets have been characterized in detail for their structural, microstructural and transport properties. α to β phase transition of Cu2Se was confirmed using temperature dependent X-ray powder diffraction and differential scanning calorimetry analyses. Scanning electron microscopy analysis reveals the presence of secondary globular nanostructures in the order of 200 nm consisting of <50 nm primary particles. High resolution transmission electron microscopy analysis confirmed the highly crystalline nature of the primary particles with irregular truncated morphology. Through a detailed investigation of different parameters in the compaction process, such as applied load, heating rate, and cooling profiles, pellets with preserved nanostructured grains were obtained. An applied load during the controlled cooling profile was demonstrated to have a big impact on the final thermoelectric efficiency of the consolidated pellets. A very high thermoelectric figure of merit (ZT) above 2 was obtained at 900 K for SPS-compacted Cu2Se nanopowders in the absence of the applied load during the controlled cooling step. The obtained ZT exceeds the state of the art in the temperature ranges above phase transition, approaching up to 25% improvement at 900 K. The results demonstrate the prominent improvement in ZT attributed both to the low thermal conductivity, as low as 0.38 W m−1 K−1 at 900 K, and the enhancement in the power factor of nanostructured Cu2Se. The proposed synthesis scheme as well as the consolidation could lead to reliable production of large scale thermoelectric nanopowders for niche applications.

**General information**

State: Published  
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Mixed Conductors, KTH - Royal Institute of Technology, Istanbul University, University of Michigan  
Authors: Tafti, M. Y. (Ekstern), Ballikaya, S. (Ekstern), Khachatourian, A. M. (Ekstern), Noroozi, M. (Ekstern), Saleemi, M. (Ekstern), Han, L. (Intern), Van Nong, N. (Intern), Bailey, T. (Ekstern), Uher, C. (Ekstern), Toprak, M. S. (Ekstern)  
Pages: 111457-111464  
Publication date: 2016  
Main Research Area: Technical/natural sciences

**Publication information**

Journal: RSC Advances  
Volume: 6  
Issue number: 112  
ISSN (Print): 2046-2069  
Ratings:  
BFI (2018): BFI-level 1  
Web of Science (2018): Indexed yes  
BFI (2017): BFI-level 1  
Scopus rating (2017): CiteScore 3.01 SJR 0.863 SNIP 0.736  
Web of Science (2017): Indexed yes  
BFI (2016): BFI-level 1  
Scopus rating (2016): CiteScore 3.06 SJR 0.889 SNIP 0.757
Properties and Structure of the LiCl-films on Lithium Anodes in Liquid Cathodes

Lithium anodes passivated by LiCl layers in different types of liquid cathodes (catholytes) based on LiAlCl₄ in SOCl₂ or SO₂ have been studied by means of impedance spectroscopy. The impedance spectra have been fitted with two equivalent circuits using a nonlinear least squares fit program. Information about the ionic conductivity and the structure of the layers has been extracted. A new physical model which is able to explain the circuit parameters is proposed. It assumes that the LiCl-layer contains a large number of narrow tunnels and cracks filled with liquid catholyte. It is explained why such tunnels probably are formed, and for a typical case it is shown that tunnels associated with most of the LiCl grain boundaries of the fine crystalline layer near the Li surface are requested in order to explain the impedance response. The LiCl production rate and through this, the growth rate of the LiCl-layer, is limited by the electron conductivity of the layer. Micro-calorimetry data parallel with impedance spectra are used for determination of the electron conductivity of the LiCl-layer.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Fundamental Electrochemistry, Technical University of Denmark
Authors: Mogensen, M. B. (Intern), Hennesø, E. (Ekstern)
Number of pages: 19
Pages: 519-534
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Acta Chimica Slovenica
Volume: 63
Issue number: 3
ISSN (Print): 1318-0207
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 0.548 SJR 0.274 CiteScore 1.01
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.27 SNIP 0.517 CiteScore 0.93
Web of Science (2016): Indexed yes
Protic Organic Ionic Plastic Crystals: Fast Solid-State Proton Conductors

High temperature polymer electrolyte membrane fuel cells (PEMFCs) operating between 100 °C and 200 °C are desirable because they offer significant benefits, such as improved electrode kinetics, simpler water and heat management, and better tolerance to fuel impurities, leading to higher overall system efficiencies [1]. However, state-of-the-art high temperature PEMFCs suffer from leakage problems associated with liquid electrolytes, such as H$_3$PO$_4$ and protic ionic liquids.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors, Technical University of Denmark
Authors: Luo, J. (Ekstern), Aili, D. (Intern), Pan, C. (Intern), Li, Q. (Intern)
Pages: 179-179
Publication date: 2016

Host publication information
Title of host publication: ISPE-XV, Uppsala 15-19th August 2016
Article number: P56
Main Research Area: Technical/natural sciences
Ptychographic X-ray computed tomography of extended colloidal networks in food emulsions

As a main structural level in colloidal food materials, extended colloidal networks are important for texture and rheology. By obtaining the 3D microstructure of the network, macroscopic mechanical properties of the material can be inferred. However, this approach is hampered by the lack of suitable non-destructive 3D imaging techniques with submicron resolution. We present results of quantitative ptychographic X-ray computed tomography applied to a palm kernel oil based oil-in-water emulsion. The measurements were carried out at ambient pressure and temperature. The 3D structure of the extended colloidal network of fat globules was obtained with a resolution of around 300 nm. Through image analysis of the network structure, the fat globule size distribution was computed and compared to previous findings. In further support, the reconstructed electron density values were within 4% of reference values.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, University of Copenhagen, Paul Scherrer Institut
Authors: Schou Nielsen, M. (Ekstern), Bøgelund Munk, M. (Ekstern), Diaz, A. (Ekstern), Pedersen, E. B. L. (Intern), Holler, M. (Ekstern), Bruns, S. (Ekstern), Risbo, J. (Ekstern), Mortensen, K. (Ekstern), Feidenhans'l, R. K. (Ekstern)
Number of pages: 8
Pages: 21-28
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Food Structure
Volume: 7
ISSN (Print): 2213-3291
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 1.38 SJR 1.019 CiteScore 2.87
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.45 SJR 1.096 SNIP 1.231
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.753 SNIP 1.158 CiteScore 2.3
BFI (2014): BFI-level 1
BFI (2013): BFI-level 1
Original language: English
3D microstructure, Colloidal network, Computed tomography, Food emulsion, X-ray phase-contrast imaging, X-ray ptychography
DOIs:
10.1016/j.foostr.2016.01.001
Links:
Source: FindIt
Source-ID: 2291817456
Publication: Research - peer-review › Journal article – Annual report year: 2016

Pulsed laser deposition of Cu$_2$ZnSnS$_4$ absorber layers assisted by a reactive sulfur beam for solar cells

General information
State: Published
Organisations: Department of Photonics Engineering, Photovoltaic Materials and Systems, Department of Energy Conversion and Storage, Technical University of Denmark
Authors: Estelrich, J. R. (Ekstern), Canulescu, S. (Intern), Traulsen, M. L. (Intern), Hansen, K. V. (Intern), Schou, J. (Intern)
Number of pages: 1
Publication date: 2016
Event: Abstract from Annual Meeting of the Danish Physical Society, Middelfart, Denmark.
Main Research Area: Technical/natural sciences
Pulsed Laser Deposition (PLD) of the Solar Cell Materials CZTS and CTS

General information
State: Published
Organisations: Department of Photonics Engineering, Photovoltaic Materials and Systems, DTU Danchip, Department of Physics, Experimental Surface and Nanomaterials Physics, Silicon Microtechnology, Department of Micro- and Nanotechnology, Department of Energy Conversion and Storage, Electrofunctional materials
Number of pages: 1
Publication date: 2016
Event: Abstract from 2016 MRS Spring Meeting & Exhibit, Phoenix, United States.
Main Research Area: Technical/natural sciences
Electronic versions:
Abstract_MRS_2016.pdf

Quantitative review of degradation and lifetime of solid oxide cells and stacks
A comprehensive review of degradation and lifetime for solid oxide cells and stacks has been conducted. Based on more than 50 parameters from 150 publications and 1 000 000 hours of accumulated testing, this paper presents a quantitative analysis of the current international status of degradation and lifetime in the field. The data is used to visualize specific trends regarding choice of materials, operating conditions and degradation rates. The average degradation rate reported is decreasing and is quickly approaching official targets. The database is published online for open-access and a continued updating by the community is encouraged. Furthermore, the commonly reported test parameters and degradation indicators are discussed. The difficulty in standardizing testing due to variations in cell and stack design, materials and intended purpose of the system is acknowledged. A standardization of reporting of long-term single-cell- and stack-tests is proposed.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry, Haldor Topsoe AS
Authors: Skafte, T. L. (Intern), Hjelm, J. (Intern), Blennow, P. (Ekstern), Graves, C. R. (Intern)
Number of pages: 19
Pages: 8-27
Publication date: 2016

Quantization of Hall Resistance at the Metallic Interface between an Oxide Insulator and SrTiO$_3$
The two-dimensional metal forming at the interface between an oxide insulator and SrTiO$_3$ provides new opportunities for oxide electronics. However, the quantum Hall effect, one of the most fascinating effects of electrons confined in two
dimensions, remains underexplored at these complex oxide heterointerfaces. Here, we report the experimental observation of quantized Hall resistance in a SrTiO$_3$ heterointerface based on the modulation-doped amorphous-LaAlO$_3$/SrTiO$_3$ heterostructure, which exhibits both high electron mobility exceeding 10,000 cm$^2$/Vs and low carrier density on the order of $\sim 10^{12}$ cm$^{-2}$. Along with unambiguous Shubnikov-de Haas oscillations, the spacing of the quantized Hall resistance suggests that the interface is comprised of a single quantum well with ten parallel conducting two-dimensional subbands. This provides new insight into the electronic structure of conducting oxide interfaces and represents an important step towards designing and understanding advanced oxide devices.

**General information**

State: Published
Organisations: Electrofunctional materials, Department of Energy Conversion and Storage, Atomic scale modelling and materials, University of Copenhagen, Max Planck Institute for Solid State Research
Number of pages: 6
Publication date: 2016
Main Research Area: Technical/natural sciences

**Publication information**

Journal: Physical Review Letters
Volume: 117
Article number: 096804
ISSN (Print): 0031-9007
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 7.58 SJR 3.622 SNIP 2.464
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 6.33 SJR 4.196 SNIP 2.61
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 4.656 SNIP 2.538 CiteScore 5.76
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 5.232 SNIP 2.71 CiteScore 6.62
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 5.675 SNIP 2.781 CiteScore 7.46
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 6.292 SNIP 2.867 CiteScore 7.19
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 6.314 SNIP 2.905 CiteScore 7.02
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 6.45 SNIP 2.757
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 6.325 SNIP 2.947
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Quantum and field effects of oxide heterostructures

The interface between two materials can show radically different properties than either of the bulk parent materials. This is not the least true for oxide interfaces, which can display multiple physical functionalities thus making them ideal for the realisation of so-called multi-plexed devices. In these multi-plexed devices, several inputs are translated into several outputs through the multiple physical functionalities. A highly prominent example of such an oxide interface is the one between LaAlO₃ and SrTiO₃. Although both LaAlO₃ and SrTiO₃ in the bulk are electrically insulating and non-magnetic, their interface nonetheless shows attractive properties such as metallic conductivity, superconductivity and ferromagnetism. This thesis will provide an extensive review of the literature concerning the interface metal found in LaAlO₃/SrTiO₃ as well as in other SrTiO₃-based heterostructures. Through this review, several open questions will be revealed, which constitute the scientific aims of this thesis. These open questions will subsequently be addressed through the work presented in the articles that were published during the course of this Ph.D. study. In the review of these published articles, the important aspects of sample preparation will initially be covered. Here, the growth of amorphous-LaAlO₃ on SrTiO₃ will be addressed in a modified pulsed laser deposition setup. This is followed by an investigation of two high-electron mobility interfaces in SrTiO₃-based heterostructures. Specifically, these interfaces are the ones between CaZrO₃/SrTiO₃ and amorphous-LaAlO₃/(La, Sr)MnO₃/SrTiO₃. The sample preparation section is ended by outlining a patterning strategy for the high-electron mobility interface at amorphous-LaAlO₃/(La, Sr)MnO₃/SrTiO₃. Subsequently, the effects of electrostatic gating is studied in two different SrTiO₃-based heterostructures. Here, it is shown that the interface between amorphous-LaAlO₃ and SrTiO₃ is superconducting with a larger critical transition temperature than that in LaAlO₃/SrTiO₃...
Rechargeable Lithium-Air Batteries: Investigation of Redox Mediators Using DEMS

The rechargeable aprotic lithium-air battery is a promising technology that offers high theoretical energy density of as much 10 times the capacity of current Li-ion batteries. This type of battery technology differs from conventional batteries because of the gas exchange during discharge/charge cycling. Characterizing the gas content during charge using Differential Electrochemical Mass Spectroscopy (DEMS) allows for in-situ characterization of chemistry in the battery.

Using our DEMS setup we have investigated different cathode materials for lithium-air batteries. A carbon black cathode exhibits a flat discharge curve with low over-potentials until the "sudden death" phenomenon which causes the voltage to drop quickly. On the charge side however, this materials exhibits significant over-potentials. These high over-potentials are linked with CO2 development which indicates that the cathode material or electrolyte is being decomposed. This is also seen with Thermally reduced Graphene Oxide (TrGO). The graphene based cathode is interesting as it exhibits a high surface area which in turn increases capacity.

Using the additive LiI, functioning as a redox mediator, the discharge curve remains largely unchanged whilst the charge curve exhibits dramatically lower over-potential, throughout the experiment [1][2]. Under certain conditions the chemistry of the battery changes, resulting in a four electron process that produces the reversible discharge product LiOH rather than Li2O2 which is observed without the redox mediator [2]. This results in higher energy densities and ideally higher cyclability due to the lower over-potentials. Using DEMS we have investigated the gas evolved in the process to determine the electron to oxygen ratio using both cathode materials mentioned.

As has been shown with lithium-air batteries the water content affects the morphology of the discharge product[3]. The effect of changing experimental conditions such as varying water content will be reported.
Relation between shape of Ni-particles and Ni migration in Ni-YSZ electrodes – a hypothesis

This is an attempt to explain a phenomenon of total depletion of Ni next to the electrolyte in Ni-YSZ cermet electrodes in solid oxide electrolysis cells during electrolysis at high current density/overpotential. Intuitively, we would think that Ni would always migrate down the steam partial pressure ($p_{H_2O}$) gradient as previously observed [1], but in the present cases Ni seems to migrate up the $p_{H_2O}$ gradient. However, it is also observed that there is a preceding phase in this Ni-YSZ electrode degradation, namely that the Ni-particles closest to the YSZ electrolyte loose contact to each other. This means that the active three phase boundary (TPB) moves away from the electrolyte and causes a significant increase in the ohmic resistance as is also observed in electrochemical impedance spectra.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Fundamental Electrochemistry, Applied Electrochemistry, Mixed Conductors
Authors: Mogensen, M. B. (Intern), Hauch, A. (Intern), Sun, X. (Intern), Chen, M. (Intern), Tao, Y. (Intern), Ebbesen, S. D. (Intern), Hendriksen, P. V. (Intern)
Number of pages: 8
Publication date: 2016

Relaxation of stresses during reduction of anode supported SOFCs

To assess the reliability of solid oxide fuel cell (SOFC) stacks during operation, the stress field in the stack must be known. During operation the stress field will depend on time as creep processes relax stresses. This work reports further details on a newly discovered creep phenomenon, accelerated creep, taking place during the reduction of a Ni-YSZ anode. This relaxes stresses at a much higher rate ($\sim 10^4$) than creep during operation. Thus, the phenomenon of accelerated creep during reduction has to be considered both in the production of stacks and in the analysis of the stress field in a stack based on anode supported SOFCs. Accelerated creep has previously been studied in experiments with simultaneous loading and reduction. The hypothesis for the phenomenon centers around a significant softening of the Ni phase, which amongst other should lead to a significant relaxation of internal stresses in the Ni(O)-YSZ microstructure. The internal residual stresses can be anticipated due the different thermal contractions of the two phases from the sintering temperature to the reduction temperature. It was thus concluded that with the recorded high creep rates, the stresses in a cell at the time of reduction should decrease significantly over minutes. In this work these internal stresses are measured in-situ before and after the reduction by use of X-ray diffraction. This is done by determining the elastic micro-strains (correlating to the stresses), which are assessed from the widening of the Bragg peaks. This enables us to determine the stresses in the different phases locally inside the microstructure of the composite Ni(O)-YSZ anode. Furthermore, the residual stresses have been modeled during cool-down from the reduction temperature. The stresses have been assessed by use of a combination of a 3D microstructural reconstruction by FIB-SEM, a microstructural finite element model and analytical homogenization considerations. A significant decrease of stresses is observed through the reduction as predicted, which partly confirms the hypothesis for the accelerated creep. Also, a significant relaxation of stresses to lower temperatures ($\sim 300^\circ C$) was also found. This was confirmed by the models, but is however not consistent with previous recorded coefficients of thermal expansion.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Imaging and Structural Analysis
Authors: Frandsen, H. L. (Intern), Chatzichristodoulou, C. (Intern), Jørgensen, P. S. (Intern), Kwok, K. (Intern), Hendriksen, P. V. (Intern)
Number of pages: 12
Pages: B11-17-B11-23
Publication date: 2016
Research and Development on Oxygen Transport Membranes at the Technical University of Denmark from Materials to Modules

Oxygen transport membranes (OTMs) are inorganic, high temperature devices that have the potential to efficiently supply oxygen to combustion processes, for example for oxy-fired (biomass) gasification or in the cement and steel industry. This work reviews aspects of material selection, design, characterization and testing of single phase and composite based OTMs that are taking place at the Technical University of Denmark (DTU). The focus will be on high performance asymmetric OTMs, in which a dense thin film oxygen separation membrane is deposited on a porous mechanically supporting layer. An OTM material should ideally have high ionic and electronic conductivity as well as good chemical stability under both oxidizing and reducing conditions. Strategies for increasing the performance by using composite dual phase membranes consisting of an ionic conductor and an electronic conductor will be discussed. Particularly membranes based on i) La0.6Sr0.4FeO3 (LSF) and CGO and ii) 10Sc1YSZ ((Y2O3)0.01(Sc2O3)0.10(ZrO2)0.89) and MnCo2O4 seem to be promising combinations and results on manufacturing and testing, including long-term results for >1500 h, of these membranes will be presented. The second part of the presentation will focus on module design and application oriented testing. Here first results from integration of OTMs into the slip stream of a biomass gasifier will be shown. Also highlights from the "Highly Efficient Tubular Membranes for Oxy-Combustion (HETMOC)" European FP7 project are included. In this project a proof-of-concept module with 25 one-end closed BCSF (BaxSr1-xCo0.8Fe0.2O3) tubes was designed and tested in a high pressure test stand designed at DTU. To maximize the partial pressure difference across the membrane, high pressure up to 5 bar was applied on the feed side and a vacuum pump was used to lower the pressure on the permeate side. Results on performance and long-term stability as well as problems encountered during the project will be presented.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Ceramic Engineering & Science
Authors: Kiebach, W. (Intern), Pirou, S. (Intern), Ovtar, S. (Intern), Bjørnetun Haugen, A. (Intern), Hendriksen, P. V. (Intern)
Publication date: 2016
Conference: PRIME 2016/230th ECS Meeting, Honolulu, United States, 02/10/2016 - 02/10/2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Electrochemical Society. Meeting Abstracts (Online)
Volume: MA2016-02
Article number: 2971
ISSN (Print): 2151-2043
Original language: English
Publication: Research - peer-review › Conference abstract in journal – Annual report year: 2016

Revealing the Origin of Activity in Nitrogen-Doped Nanocarbons towards Electrocatalytic Reduction of Carbon Dioxide

Carbon nanotubes (CNTs) are functionalized with nitrogen atoms for reduction of carbon dioxide (CO2). The investigation explores the origin of the catalyst's activity and the role of nitrogen chemical states therein. The catalysts show excellent performances, with about 90% current efficiency for CO formation and stability over 60 hours. The Tafel analyses and density functional theory calculations suggest that the reduction of CO2 proceeds through an initial rate-determining transfer of one electron to CO2, which leads to the formation of carbon dioxide radical anion (CO2C). The initial reduction barrier is too high on pristine CNTs, resulting in a very high overpotentials at which the hydrogen evolution reaction dominates over CO2 reduction. The doped nitrogen atoms stabilize the radical anion, thereby lowering the initial reduction barrier and improving the intrinsic activity. The most efficient nitrogen chemical state for this reaction is quaternary nitrogen, followed by pyridinic and pyrrolic nitrogen.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors, Chinese Academy of Sciences, Huaiyin Normal University, University of Messina
Authors: Xu, J. (Ekstern), Kan, Y. (Ekstern), Huang, R. (Ekstern), Zhang, B. (Ekstern), Wang, B. (Ekstern), Wu, K. (Ekstern), Lin, Y. (Ekstern), Sun, X. (Ekstern), Li, Q. (Intern), Centi, G. (Ekstern), Su, D. (Ekstern)
Reversible Decomposition of Secondary Phases in BaO Infiltrated LSM Electrodes—Polarization Effects

In operando Raman spectroscopy is used to study ceramic La$_{0.85}$Sr$_{0.15}$MnO$_{3-\delta}$ electrodes infiltrated with BaO. The aim of this work is to clarify why BaO infiltration reduces the polarization resistance in oxygen containing atmospheres. Prior to the in operando experiments, ex situ X-ray diffraction and Raman spectroscopy reveal the formation of a secondary phase, Ba$_3$Mn$_2$O$_8$, on the electrode. During the in operando Raman investigation of the BaO-infiltrated La$_{0.85}$Sr$_{0.15}$MnO$_{3-\delta}$ electrodes, experiments are performed at 300 and 500 °C with oxygen partial pressure 0.1 atm and with −1 or +1 V applied potential. A changing electrode surface is observed during operation as the Ba$_3$Mn$_2$O$_8$ secondary phase decomposes and manganese oxide accumulates on the electrode surface during cathodic polarization. The observed changes are reversible. These results suggest that the formation of Ba$_3$Mn$_2$O$_8$ is responsible for the reduced polarization resistance observed at open circuit voltage (OCV) in an oxygen containing atmosphere. Furthermore, the results illustrate the dramatic differences between the electrode surface composition at OCV and during cathodic polarization. Overall, the results highlight the dynamic interactions between minor secondary phases and applied potential, a general effect that may be important for the high-performance frequently observed with ceramic electrodes prepared by infiltration.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Fundamental Electrochemistry, Imaging and Structural Analysis, Electrofunctional materials, Montana State University
Authors: Traulsen, M. L. (Intern), McIntyre, M. D. (Ekstern), Norrman, K. (Intern), Sanna, S. (Intern), Mogensen, M. B. (Intern), Walker, R. A. (Ekstern)
Number of pages: 11
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Advanced Materials Interfaces
Article number: 1600750
ISSN (Print): 2196-7350
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 4.13 SJR 1.796 SNIP 0.785
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.57 SJR 1.545 SNIP 0.876
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.193 SNIP 0.668 CiteScore 2.47
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
BFI (2013): BFI-level 1
Original language: English
Electronic versions:
Reversible Decomposition of Secondary Phases. Embargo ended: 29/11/2017
Supporting Information. Embargo ended: 29/11/2017
DOIs:
10.1002/admi.201600750
Source: FindIt
Source-ID: 2349355776
Publication: Research - peer-review › Journal article – Annual report year: 2016

Reversible Operation of Solid Oxide Cells for Sustainable Fuel Production and Solar/Wind Load-Balancing
The solid oxide electrochemical cell (SOC) is a promising candidate for large-scale energy storage. In electrolysis mode it stores renewable electricity as chemical energy in the form of fuels like hydrogen and hydrocarbons, and the same cell can be operated in the reversedirection to produce electricity from fuels – either previously stored fuels or from an external supply e.g. natural gas or biogas. This reversibility combined with fuel-flexibility is unique among energy storage technologies like closed-system batteries and single-direction electrolyzers. However, few studies have been conducted with focus on fundamentals or applications of bi-directional operation. This presentation will highlight our recent
developments in applying reversible SOCs (RSOCs) for renewable energy storage with respect to cell and stack testing, cell and system design, and techno-economic analysis. At the cell level, long-term testing has shown that improved stability can be achieved by reversible operation compared with steady-state electrolysis operation. Further, we have developed novel Ni-free fuel electrodes that both outperform conventional Ni-based electrodes and do not catalyze carbon deposition, which opens the door to advanced applications of RSOCs that utilize carbonaceous fuels. At the stack level, we have demonstrated operation that follows real-world time-series electricity supply and demand data, considering a 100% renewable energy scenario where wind power is the only power supply. When the wind power supply exceeds demand, the RSOC stack produces syngas via co-electrolysis of CO2 and H2O. Part of the syngas is converted to methanol downstream in the system to meet the demand of transportation vehicles, and the rest is stored for electrical load balancing by conversion back to electricity in fuel cell mode when electricity demand exceeds the wind power supply. At the system level, techno-economic analyses and system designs for different scales and applications have been realized. A simulation of an RSOC system that uses real-world time-series market prices for electricity and natural gas in Denmark to decide when to operate in electrolysis mode (buying electricity and selling methane) or fuel-cell mode (buying gas and selling electricity) shows the advantage of a reversible system and the changing operating profile as the fraction of wind power supply grows. Finally, we discuss the potential for systems with novel chemistries and components to compete with state-of-the-art rechargeable batteries with respect to cost and round-trip efficiency.

General information
State: Published
Authors: Graves, C. R. (Intern), Villarreal, D. (Ekstern), Mýrdal, J. S. G. (Intern), Jensen, S. H. (Intern), Hendriksen, P. V. (Intern), Mogensen, M. B. (Intern)
Publication date: 2016
Conference: PRiME 2016/230th ECS Meeting, Honolulu, United States, 02/10/2016 - 02/10/2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Electrochemical Society. Meeting Abstracts (Online)
Volume: MA2016-02
Article number: 3075
ISSN (Print): 2151-2043
Original language: English
Links: http://ma.ecsdl.org/content/MA2016-02/40/3075.abstract?sid=d44335da-e553-4ef7-99db-ef6a481c38d2
Publication: Research - peer-review » Conference abstract in journal – Annual report year: 2016

Role of Stress Factors on the Adhesion of Interfaces in R2R Fabricated Organic Photovoltaics
The role of the common stress factors such as high temperature, humidity, and UV irradiation on interface adhesion of roll-to-roll fabricated organic photovoltaic (OPV) devices is investigated. The samples range from bare front electrodes to complete devices. It is shown that applying single stress or combinations of stresses onto the samples variably affect the adhesion properties of the different interfaces in the OPV device. It is revealed that while the exposure of the complete devices to the stresses results in the loss of photovoltaic performance, some interfaces in the devices present improved adhesion properties. Depth profiling analysis on the fractured samples reveals interdiffusion of layers in the structure, which results in the increase of adhesion and change of the debond path. It is shown that through diffusion and intermixing of internal interfaces coupled stresses can increase the adhesion of OPV interfaces by over tenfold. The results are additionally compared to the photovoltaic performance of the complete devices.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Functional organic materials, Stanford University
Authors: Corazza, M. (Intern), Rolston, N. (Ekstern), Dauskardt, R. H. (Ekstern), Beliatis, M. (Intern), Krebs, F. C. (Intern), Gevorgyan, S. (Intern)
Number of pages: 7
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Advanced Energy Materials
Article number: 1501927
ISSN (Print): 1614-6832
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
In this paper, we investigate three diketopyrrolopyrrole (DPP) based small molecular non-fullerene acceptors, namely Ph(DPP)3, Ph(DPP)2, and PhDMe(DPP)2, focusing on molecular geometry effects on the frontier orbital level, light absorption, molecular configuration, electron mobility, thin film morphology, and photovoltaic performance of both spin-coated ITO based and roll coated large area, ITO- and vacuum-free organic solar cells (OSCs). For spin-coated devices based on P3HT as the donor polymer the solar cells gave power conversion efficiencies (PCEs) in the following order for (P3HT:PhDMe(DPP)2, 0.65%) > (P3HT:Ph(DPP)2, 0.48%) > (P3HT:Ph(DPP)3, 0.31%). All devices present an open circuit voltage (Voc) higher than 1.0 V. For the roll-coated devices, the PCEs were found to fall in another order and with lower values (P3HT:Ph(DPP)3, 0.54%) > (P3HT:Ph(DPP)2, 0.43%) > (P3HT:PhDMe(DPP)2, 0.04%) and the highest Voc was 0.82 V. Our preliminary results highlight the influence of geometry, structure and processing on the performance of non-fullerene acceptors.
Scopus rating (2017): CiteScore 3.01 SJR 0.863 SNIP 0.736
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.06 SJR 0.889 SNIP 0.757
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.947 SNIP 0.834 CiteScore 3.42
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.113 SNIP 0.962 CiteScore 3.87
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.119 SNIP 0.904 CiteScore 3.74
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Scopus rating (2012): SJR 0.872 SNIP 0.619 CiteScore 2.4
ISI indexed (2012): ISI indexed no
Web of Science (2012): Indexed yes
Original language: English
DOIs:
10.1039/c6ra06898g
Source: FindIt
Source-ID: 2303730516
Publication: Research - peer-review › Journal article – Annual report year: 2016

Roll-coating fabrication of flexible organic solar cells: comparison of fullerene and fullerene-free systems
Flexible organic solar cells (OSCs) based on a blend of low-bandgap polymer donor PTB7-TH and nonfullerene small molecule acceptor IEIC were fabricated via a roll-coating process under ambient atmosphere. Both an indium tin oxide (ITO)-free substrate and a flexible ITO substrate were employed in these inverted OSCs. OSCs with flexible ITO and ITO-free substrates exhibited power conversion efficiencies (PCEs) up to 2.26% and 1.79%, respectively, which were comparable to those of the reference devices based on fullerene acceptors under the same conditions. This is the first example for all roll-coating fabrication procedures for flexible OSCs based on non-fullerene acceptors with the PCE exceeding 2%. The fullerene-free OSCs exhibited better dark storage stability than the fullerene-based control devices.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Functional organic materials, Peking University
Pages: 1044-1051
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Materials Chemistry A
Volume: 4
ISSN (Print): 2050-7488
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 9.61 SJR 3.488 SNIP 1.55
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 8.46 SJR 3.075 SNIP 1.479
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 2.62 SNIP 1.643 CiteScore 8.36
Roll-to-Roll Printed Electronics for Standalone Smart Windows

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Organic Energy Materials
Authors: Pastorelli, F. (Intern)
Number of pages: 1
Publication date: 2016
Event: Abstract from 2016 MRS Fall Meeting & Exhibit, Boston, MA, United States.
Main Research Area: Technical/natural sciences
Electronic versions:
Roll_to_Roll_Printed_Electronics.pdf

Bibliographical note
Symposium PMS : Hierarchical, Hybrid and Roll-to-Roll Manufacturing for Device Applications
Source: PublicationPreSubmission
Source-ID: 127807130
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2016

Roll-to-roll printed silver nanowires for increased stability of flexible ITO-free organic solar cell modules
We report the use of roll-to-roll printed silver nanowire networks as front electrodes for fully roll-to-roll processed flexible indium-tin-oxide (ITO) free OPV modules. We prepared devices with two types of back electrodes, a simple PEDOT:PSS back electrode and a PEDOT:PSS back electrode with a printed silver grid in order to simultaneously explore the influence of the back electrode structure on the operational stability of the modules that did not include any UV-protection. We subjected the devices to stability testing under a number of protocols recommended by the international summit on OPV stability (ISOS). We explored accelerated ISOS-D-2, ISOS-D-3, ISOS-L-2, ISOS-L-3, ISOS-O-1 and ISOS-O-2 testing protocols and compared the performance to previous reports employing the same testing protocols on devices with PEDOT:PSS instead of the silver nanowires in the front electrode. We find significantly increased operational stability across all ISOS testing protocols over the course of the study and conclude that replacement of PEDOT:PSS in the front electrode with silver nanowires increase operational stability by up to 1000%. The duration of the tests were in the range of 140–360 days. The comparison of front and back electrode stability in this study shows that the modules with silver nanowire front electrodes together with a composite back electrode comprising PEDOT:PSS and a silver grid present the best operational stability.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Functional organic materials
Number of pages: 9
Pages: 318-326
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Nanoscale
Volume: 8
ISSN (Print): 2040-3364
Ratings:
Ruled-based control of off-grid electrolysis

This work deals with a ruled-based control strategy to produce hydrogen from wind and wave energy in an offshore platform. These renewable energies feed a set of alkaline electrolyzers that produce H2. The proposed control system allows regulating the operation of the electrolyzers, taking into account the energy available and optimizing the performance of the plant. Simulation results obtained are presented, showing correct operation of the platform under this proposed control.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, University of Valladolid, Universidade Federal de Santa Catarina
Authors: Serna, A. (Ekstern), Tadeo, F. (Ekstern), Normey-Rico, J. E. (Ekstern), Agersted, K. (Ekstern)
Pages: 1114-1115
Publication date: 2016

Host publication information
Title of host publication: Proceedings of the 21st World Hydrogen Energy Conference (WEC 2016)
Publisher: Spanish Hydrogen Association
Main Research Area: Technical/natural sciences
Conference: The 21st World Hydrogen Energy Conference (WHEC), Zaragoza, Spain, 13/06/2016 - 13/06/2016
Publication: Research - peer-review › Article in proceedings – Annual report year: 2017

Scandium-doped zinc cadmium oxide as a new stable n-type oxide thermoelectric material

Scandium-doped zinc cadmium oxide (Sc-doped ZnCdO) is proposed as a new n-type oxide thermoelectric material. The material is sintered in air to maintain the oxygen stoichiometry and avoid instability issues. The successful alloying of CdO
with ZnO at a molar ratio of 1 : 9 significantly reduced the thermal conductivity by up to 7-fold at room temperature. By carefully selecting the Sc-dopant concentrations, a high power factor of \( 7.1 \times 10^{-4} \, \text{W m}^{-1} \text{K}^{-2} \) at 1173 K could be obtained. Therefore, the highest ZT = 0.3 at 1173 K was achieved for the Zn\(_{0.9} \text{Cd}_{0.1} \text{Sc}_{0.01} \text{O}_{1.015} \) sample, and it has so far one of the highest ZT values among those reported for ZnO based thermoelectric materials over the temperature range, e.g., its ZT value at 300 K, which is 0.012, is over 1 order of magnitude higher than that of the state-of-the-art nanostructured Al-doped ZnO, which is 0.0013. It suggests that this material is a good candidate for improving the overall conversion efficiencies in oxide thermoelectric modules. Meanwhile, Sc-doped ZnCdO is robust in air at high temperatures, whereas other n-type materials, such as Al-doped ZnO, will experience rapid degradation of their electrical conductivity and ZT.
Self-Assembled Plasmonic Nanoparticles for Organic Photovoltaics

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Organic Energy Materials
Authors: Pastorelli, F. (Intern)
Number of pages: 1
Publication date: 2016
Event: Abstract from 2016 MRS Fall Meeting & Exhibit, Boston, MA, United States.
Main Research Area: Technical/natural sciences
Electronic versions:
Self_Assembled_Plasmonic_Nanoparticles.pdf

Bibliographical note
Symposium EM7 : Functional Plasmonics
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2016

Self-supported ceramic substrates with directional porosity by mold freeze casting

Manufacture of thin-film ceramic substrates with high permeability and robustness is of high technological interest. In this work thin (green state thickness ~500 μm) porous yttria-stabilized zirconia self-supported substrates were fabricated by pouring stable colloidal aqueous suspensions in a mold and applying directional freeze casting. Use of optimized suspension, cryoprotector additive and mold proved to deliver defect free ceramic films with high dimensional control. Microstructure analysis demonstrated the formation of desirable aligned porosity at macro-structural scale and resulted to be highly dependent on colloidal behaviour and freeze casting conditions. Manufactured green films were joined by lamination at room temperature and sintered to obtain symmetrical cells consisting of two porous self-supported substrate electrodes (~420 μm) and dense yttria stabilized zirconia electrolyte (~10 μm).

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Applied Electrochemistry , CSIC
Authors: Gurauskis, J. (Intern), Graves, C. R. (Intern), Moreno, R. (Ekstern), Nieto, M. (Ekstern)
Number of pages: 7
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of the European Ceramic Society
Volume: 37
Issue number: 2
ISSN (Print): 0955-2219
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 3.55 SJR 1.068 SNIP 1.698
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.25 SJR 1.142 SNIP 1.888
Web of Science (2016): Indexed yes
Shaping our energy future by electrospinning

Electrospinning is the most versatile technique to design nanofiber materials with numerous applications in the fields of filtration, membranes, catalysts, reinforcement and biomedicals. Using electrospinning, we are able to design a complex structure from a rich variety of materials including polymers, metals, ceramics and composite, with the ability to control composition, morphology and secondary structure and tailor performance and functionality for specific applications. Moreover, with significant improvement in electrospinning equipment design, industrial-scale electrospinning technologies with production rate of several thousands of square meters per day are transforming advanced material research done in our labs into products serving our everyday life.

This talk will show you the power of electrospinning technology with exciting projects that address the sizable challenges in energy devices by electrospinning. The outcomes of these unique nanofibrous structures are significant improvements...
Silicon doped InP as an alternative plasmonic material for mid-infrared

Silicon-doped InP is grown on top of semiinsulating iron-doped and sulfur-doped InP substrates by metalorganic vapor phase epitaxy (MOVPE), and the growth parameters are adjusted to obtain various free carrier concentrations from $1.05 \times 10^{19}$ cm$^{-3}$ up to $3.28 \times 10^{19}$ cm$^{-3}$. Midinfrared (IR) reflection spectra of the samples with different carrier concentrations are used to retrieve pertaining dielectric functions as the key factor for understanding plasmonic behavior of InP:Si in the mid-IR wavelength range.

Simulation, design and proof-of-concept of a two-stage continuous hydrothermal flow synthesis reactor for synthesis of functionalized nano-sized inorganic composite materials

Computational fluid dynamics simulations were employed to evaluate several mixer geometries for a novel two-stage continuous hydrothermal flow synthesis reactor. The addition of a second stage holds the promise of allowing the synthesis of functionalized nano-materials as for example core-shell or decorated particles. Based on the simulation results, a reactor system employing a confined jet mixer in the first and a counter-flow mixer in the second stage was designed and built. The two-stage functionality and synthesis capacity is shown on the example of single- and two-stage syntheses of pure and mixed-phase NiO and YSZ particles.
Slot-Die-Coated V$_2$O$_5$ as Hole Transport Layer for Flexible Organic Solar Cells and Optoelectronic Devices

Vanadium pentoxide has been proposed as a good alternative hole transport layer for improving device lifetime of organic photovoltaics. The article presents a study on the optimization of slot-die-coated vanadium oxide films produced with a roll coating machine with the aim of achieving scalable organic solar cells and photo-detectors with improved performance. The effect of different diluents on the electrical properties of the vanadium oxide films is investigated, and methodologies for efficient interfacing of the anode are studied. Furthermore, the lifetime of the cells with incorporated vanadium oxide is investigated employing different encapsulation methods. Finally, an application of the manufactured scalable devices in proximity sensors is demonstrated using a 3D-printed scaffold.

General information

State: Published
Organisations: Department of Energy Conversion and Storage, Functional organic materials
Number of pages: 10
Pages: 1494-1503
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information

Journal: Advanced Energy Materials
Volume: 18
Issue number: 8
ISSN (Print): 1614-6832
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 16.78 SJR 8.23 SNIP 2.347
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 12.96 SJR 6.515 SNIP 2.14
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 6.219 SNIP 2.546 CiteScore 14.2
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 6.668 SNIP 2.942 CiteScore 15.27
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 6.006 SNIP 2.949 CiteScore 13.24
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Scopus rating (2012): SJR 5.575 SNIP 2.181 CiteScore 9.64
ISI indexed (2012): ISI indexed no
ISI indexed (2011): ISI indexed no
Web of Science (2011): Indexed yes
Original language: English
DOIs: 10.1002/adem.201600119

Space-Confined Synthesis of Three-Dimensional Boron/Nitrogen-Doped Carbon Nanotubes/Carbon Nanosheets Line-in-Wall Hybrids and Their Electrochemical Energy Storage Applications

This research demonstrates a flexible one-pot strategy for fabricating three-dimensional (3D) boron/nitrogen-doped networks of carbon nanotubes(CNTs)/carbon nanosheets "Line-in-Wall" hybrids (LIWNB) based on the space-confined
template method. In the synthesis, the high rate of freezing step and freeze-dried process enable the CNTs and carbon-heteroatoms sources confined in the limited space of the self-assembled NaCl salts, which are then heat-treated to obtain a B/N-doped network constructed by "Line-in-Wall" type of carbon hybrids. By combining the 3D B/N-doped carbon nanosheets network and CNTs in this unique pattern, the LIW-NB integrates advantages of three aspects: first, the doped heteroatoms enhancing electrochemical properties of carbon matrix; second, the warp-proof nanosheets supplying high specific surface area; and the extracted and embedded CNTs serving as electron conductive paths and reinforcing the whole architecture. As a result, the 3D LIW-NB shows excellent electrochemical properties: as the electrode of supercapacitors, LIW-NB exhibits high specific capacity at different current densities (389 F g⁻¹ at 1 A g⁻¹ and 129 F g⁻¹ at 20 A g⁻¹); as the lithium ion battery anode, it possesses high reversible storage capacity (1165 mAh g⁻¹ at 0.1 A g⁻¹) and stable long cycle performance at high rate (1000 cycles at 2 A g⁻¹).
Specific electrical conductivity in molten potassium dihydrogen phosphate $\text{KH}_2\text{PO}_4$ - An electrolyte for water electrolysis at $\sim$300°C

The conductivity of pure molten $\text{KH}_2\text{PO}_4$ salt and four mixtures with more or less water ($\text{KH}_2\text{PO}_4$-$\text{H}_2\text{O}$ and $\text{KH}_2\text{PO}_4$-KPO$_3$ systems, respectively) were measured at temperatures of 240-320°C and under their own water vapor pressures. Molten $\text{KH}_2\text{PO}_4$ has been proven to be a promising electrolyte for an elevated temperature pressurized water electrolyzer demonstrating high conductivity of $\sim$0.30 Scm$^{-1}$ at 300°C. The conductivity data are given as polynomial functions of temperature and composition. The melting point of the pure salt under its own water vapor pressure was determined to be $\sim$272°C.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors, Department of Chemistry
Authors: Nikiforov, A. V. (Intern), Berg, R. W. (Intern), Petrushina, I. (Intern), Bjerrum, N. J. (Intern)
Number of pages: 6
Pages: 545-550
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Applied Energy
Volume: 175
ISSN (Print): 0306-2619
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 8.44 SJR 3.162 SNIP 2.765
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 7.78 SJR 3.011 SNIP 2.61
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Stability and Polaronic Motion of Self-Trapped Holes in Silver Halides: Insight through DFT plus U Calculations

Polarons and their associated transport properties are a field of great current interest both in chemistry and physics. To further our understanding of these quasi-particles, we have carried out first-principles calculations of self-trapped holes (STHs) in the model compounds AgCl and AgBr, for which extensive experimental information exists. Our calculations confirm that the STH solely stabilizes in AgCl but with a binding energy of only 165 meV, an order of magnitude smaller...
than that found for the V\textsubscript{K} center in KCl. Key contributions to this stabilization energy come from the local relaxation along breathing (\epsilon_{1g}) and Jahn Teller (\epsilon_{eg}) modes in the AgCl\textsubscript{6}\textsuperscript{4+} unit. To study the transfer of the STH among silver sites, we (i) use first-principles calculations to obtain the hopping barrier of the STH to first and second neighbors, involving eight distinct paths, using first-principles and (ii) construct a simple model, based on Slater-Koster parameters, that highlights the similarity of polaron transfer with magnetic superexchange. This allows one understanding of why the movement of STHs to second neighbors is highly enhanced with respect to closer ones. In agreement with experimental data and the model, the present calculations prove the existence of a dominant mechanism of polaronic motion that corresponds to the displacement of the STHs to the next-nearest sites in the <100> direction and a small barrier of 37 meV. This mechanism is dominated by the covalency inside a Ag\textsubscript{2}X\textsubscript{6}\textsuperscript{4+} complex (X:Cl;Br), thus explaining why the STH is not stabilized in AgBr following the increase of covalent due to the Cl -> Br substitution. The present calculations confirm that, similar to 10% of the charge associated with the STH in AgCl is outside the AgCl\textsubscript{6}\textsuperscript{4+} complex. This fact is behind the differences between optical and magnetic properties of the STH in AgCl and those observed in KCl:Ag\textsuperscript{2+}.

**General information**

State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, University of Cantabria
Authors: Loftager, S. (Intern), Garcia-Fernandez, P. (Ekstern), Aramburu, J. A. (Ekstern), Moreno, M. (Ekstern), Garcia Lastra, J. M. (Intern)
Number of pages: 16
Pages: 8509-8524
Publication date: 2016
Main Research Area: Technical/natural sciences

**Publication information**

Journal: Journal of Physical Chemistry C
Volume: 120
Issue number: 16
ISSN (Print): 1932-7447
Ratings:
- BFI (2018): BFI-level 1
- Web of Science (2018): Indexed yes
- BFI (2017): BFI-level 1
- Scopus rating (2017): CiteScore 4.58 SJR 2.135 SNIP 1.147
- Web of Science (2017): Indexed yes
- BFI (2016): BFI-level 1
- Scopus rating (2016): CiteScore 4.48 SJR 1.964 SNIP 1.195
- Web of Science (2016): Indexed yes
- BFI (2015): BFI-level 1
- Scopus rating (2015): SJR 1.886 SNIP 1.26 CiteScore 4.68
- Web of Science (2015): Indexed yes
- BFI (2014): BFI-level 1
- Scopus rating (2014): SJR 2.032 SNIP 1.447 CiteScore 5.08
- Web of Science (2014): Indexed yes
- BFI (2013): BFI-level 1
- Scopus rating (2013): SJR 2.143 SNIP 1.445 CiteScore 5.14
- ISI indexed (2013): ISI indexed yes
- Web of Science (2013): Indexed yes
- BFI (2012): BFI-level 1
- Scopus rating (2012): SJR 2.529 SNIP 1.461 CiteScore 4.98
- ISI indexed (2012): ISI indexed yes
- Web of Science (2012): Indexed yes
- BFI (2011): BFI-level 1
- Scopus rating (2011): SJR 2.339 SNIP 1.465 CiteScore 4.92
- ISI indexed (2011): ISI indexed yes
- Web of Science (2011): Indexed yes
- BFI (2010): BFI-level 1
- Scopus rating (2010): SJR 2.462 SNIP 1.362
- Web of Science (2010): Indexed yes
Stability of MOF-5 in a hydrogen gas environment containing fueling station impurities

Metal-organic frameworks (MOFs) are an emerging class of porous, crystalline materials with potential application as hydrogen storage media in fuel cell vehicles. Unlike lower capacity adsorbents such as zeolites and carbons, some MOFs are expected to degrade due to attack by impurities present in the hydrogen fuel stream. Hydrogen intended for use in fuel cell vehicles should satisfy purity standards, such as those outlined in SAE J2719. This standard limits the concentration of certain species in the fuel stream based primarily on their deleterious effects on PEM fuel cells. However, the impact of these contaminants on MOFs is mostly unknown. In the present study MOF-5 is adopted as a prototypical moisture-sensitive hydrogen storage material. Five "impure" gas mixtures were prepared by introducing low-to-moderate levels (i.e., up to ~200 times greater than the J2719 limit) of selected contaminants (NH₃, H₂S, HCl, H₂O, CO, CO₂, CH₄, O₂, N₂, and He) to pure hydrogen gas. Subsequently, MOF-5 was exposed to these mixtures over hundreds of adsorption/desorption pressure-swing cycles and for extended periods of static exposure. The impact of exposure was assessed by periodically measuring the hydrogen storage capacity of an exposed sample. Hydrogen chloride was observed to be the only impurity that yielded a measurable, albeit small, decrease in hydrogen capacity; no change in H₂ uptake was observed for the other impurities. Post-cycling and post-storage MOF-5 samples were also analyzed using infrared spectroscopy and x-ray diffraction. These analyses reveal slight changes in the spectra for those samples exposed to HCl and NH₃ compared to the pristine material. These measurements suggest that MOF-5 – and likely many other MOFs – exhibit sufficient robustness to withstand prolonged exposure to ‘off-spec’ hydrogen fuel.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, University of Michigan, Ford Motor Company, BASF
Authors: Ming, Y. (Ekstern), Purewal, J. (Ekstern), Yang, J. (Ekstern), Xu, C. (Ekstern), Veensta, M. (Ekstern), Gaab, M. (Ekstern), Müller, U. (Ekstern), Siegel, D. J. (Intern)
Pages: 9374–9382
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Volume: 41
Issue number: 22
ISSN (Print): 0360-3199
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Strain development during the phase transition of La(Fe,Mn,Si)_{13}H_z

We use powder X-ray diffraction to evaluate the temperature dependence of the crystalline properties during the magnetic phase transition of La(Fe,Mn,Si)_{13}H_z as a function of the Fe/Mn/Si ratio. Both the paramagnetic and ferromagnetic
phases were observed as peak overlaps in the patterns around the Curie temperature ($T_C$) occurring continuously in a
temperature range of about 5 K around $T_C$. Using the Williamson-Hall method, we evaluate the strain developing in the
crystallites during the transition and find that it is associated with the growth of the paramagnetic phase as the transition
occurs. Based on our measurements and microstructure analyses, we propose that cracking during the phase transition is
due to or aggravated by the small content of a La-rich phase.

General information
State: Published
Organisations: Electrofunctional materials, Department of Energy Conversion and Storage, Atomic scale modelling and
materials, Department of Chemistry, X-ray Crystallography
Authors: Neves Bez, H. (Intern), Nielsen, K. K. (Intern), Smith, A. (Intern), Norby, P. (Intern), Ståhl, K. (Intern), Bahl, C. R.
H. (Intern)
Number of pages: 4
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Volume: 109
Issue number: 5
Article number: 051902
ISSN (Print): 0003-6951
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 3.25 SJR 1.382 SNIP 1.167
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.67 SJR 1.673 SNIP 1.249
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.499 SNIP 1.226 CiteScore 2.47
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.861 SNIP 1.492 CiteScore 3.25
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.146 SNIP 1.633 CiteScore 3.77
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 2.57 SNIP 1.739 CiteScore 3.76
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 2.814 SNIP 1.917 CiteScore 4.04
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 2.92 SNIP 1.775
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.826 SNIP 1.834
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 2.894 SNIP 1.82
Web of Science (2008): Indexed yes
Study of multi-layer active magnetic regenerators using magnetocaloric materials with first and second order phase transition: Paper

Magnetocaloric materials (MCM) with a first order phase transition (FOPT) usually exhibit a large, although sharp, isothermal entropy change near their Curie temperature, compared to materials with a second order phase transition (SOPT). Experimental results of applying FOPT materials in recent magnetocaloric refrigerators (MCR) demonstrated the great potential for these materials, but a thorough study on the impact of the moderate adiabatic temperature change and strong temperature dependence of the magnetocaloric effect (MCE) is lacking. Besides, comparing active magnetic regenerators (AMR) using FOPT and SOPT materials is also of fundamental interest. We present modeling results of multi-layer AMRs using FOPT and SOPT materials based on a 1D numerical model. First the impact of isothermal entropy change, adiabatic temperature change and shape factor describing the temperature dependence of the MCE are quantified and analyzed by using artificially built magnetocaloric properties. Then, based on measured magnetocaloric properties of La(Fe,Mn,Si)13H y and Gd, an investigation on how to layer typical FOPT and SOPT materials with different temperature spans is carried out. Moreover, the sensitivity of variation in Curie temperature distribution for both groups of AMRs is investigated. Finally, a concept of mixing FOPT and SOPT materials is studied for improving the stability of layered AMRs with existing materials.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Authors: Lei, T. (Intern), Engelbrecht, K. (Intern), Nielsen, K. K. (Intern), Neves Bez, H. (Intern), Bahl, C. (Intern)
Number of pages: 10
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Volume: 49
Issue number: 34
Article number: 345001
ISSN (Print): 0022-3727
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
Study of the Polarization Behavior of $\text{Ce}_{0.9}\text{Gd}_{0.1}\text{O}_{2-\delta}$ Single Crystals below 350°C to Room Temperature

Single crystalline ceria samples with the composition $\text{Ce}_{0.9}\text{Gd}_{0.1}\text{O}_{2-\delta}$ were pre-polarized with ±5 V for up to 300 s using a Pt coated AFM tip as working electrode. The direct contact zone had a diameter of <50 nm. Subsequently, the effect of the polarization on the surface potential of the samples was investigated by mapping the introduced defect gradient and its decay with time using Kelvin probe force microscopy. The generated surface potential gradients were found to have a diameter of up to 1 μm, which is explained by the local ionization of defect associates by the applied high electric field.

Measurements were performed at room temperature and 50°C. The polarization behavior of the $\text{Ce}_{0.9}\text{Gd}_{0.1}\text{O}_{2-\delta}$ single crystals was compared to cyclovoltammetry and polarization-relaxation experiments at $T \leq 350°C$ and in dry air or nitrogen which were performed using a specially suited AFM (Controlled Atmosphere High Temperature Scanning Probe Microscope CAHT-SPM by Semilab).

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Imaging and Structural Analysis, Department of Chemistry, University of Munster, Technische Universität Berlin
Number of pages: 7
Pages: H1179-H1185
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Electrochemical Society. Journal
Volume: 163
Issue number: 14
ISSN (Print): 0013-4651
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 3.48 SJR 1.267 SNIP 1.009
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.97 SJR 1.222 SNIP 0.963
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.115 SNIP 1.066 CiteScore 3.17
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.213 SNIP 1.25 CiteScore 3.36
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.169 SNIP 1.309 CiteScore 2.92
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.329 SNIP 1.281 CiteScore 2.61
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.331 SNIP 1.335 CiteScore 2.74
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Study of variables for accelerating lifetime testing of SOFCs

Solid oxide fuel cell (SOFC) applications require lifetimes of several years on the system level. A big challenge is to proof/confirm/demonstrate such exceptionally long lifetimes. Accelerated or compressed testing are possible methods. Activities in this area have been carried out without arriving at a generally accepted result. First accelerated testing approaches were performed under non-steady operation conditions (current cycling, temperature cycling) by different researchers [1, 2]. However, cycling conditions seemed to have no significant impact on degradation mechanisms. Furthermore, tests done at different current load cycling profiles revealed a strong deviation between predicted and measured lifetime [3]. In this study, we present a detailed analysis of durability results for degradation mechanisms of single SOFC components as function of operating conditions. Electrochemical impedance data is collected and used to de-convolute the individual losses of single SOFC cell components – electrolyte, cathode and anode. The obtained knowledge is adopted to identify operation profiles and appropriate stresses in order to execute appropriate accelerated testing for lifetime investigation of SOFCs.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry
Authors: Ploner, A. (Intern), Hagen, A. (Intern), Hauch, A. (Intern)
Number of pages: 1
Publication date: 2016
Event: Abstract from 12th European SOFC & SOE Forum, Lucerne, Switzerland.
Main Research Area: Technical/natural sciences
Electronic versions:
Subsolidus Phase Relations of the CaO-REOx-CuO Systems (RE = Eu, Tb, Dy, Ho, Er, Lu and Sc) at 900 °C in Air

The subsolidus phase relations of the CaO-REOx-CuO systems (RE = Eu, Tb, Dy, Ho, Er, Lu and Sc) were investigated in air at 900 °C. The pseudo-ternary sections with RE = Tb, Dy, Ho, Er and Lu have a similar structure. They have in common with the RE = Eu system a solid solution of Ca0.833−xRExCuO2+y composition but the system with RE = Eu differs by the presence of an Eu2CuO4 phase instead of RE2Cu2O5 for RE = Tb, Dy, Ho, Er and Lu. In contrast, the CaO-ScO1.5-CuO section does not contain a Ca0.833−xScxCuO2+y solid solution and is dominated by the CaSc2O4 phase, which has no equivalent in the other systems at 900 °C in air.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Authors: Grivel, J. (Intern)
Number of pages: 10
Pages: 601-610
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Phase Equilibria and Diffusion
Volume: 37
Issue number: 5
ISSN (Print): 1547-7037
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 1.12 SJR 0.575 SNIP 0.864
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 0.85 SJR 0.472 SNIP 0.709
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.363 SNIP 0.527 CiteScore 0.64
Web of Science (2015): BFI-level 1
Scopus rating (2014): SJR 0.373 SNIP 0.635 CiteScore 0.73
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.33 SNIP 0.552 CiteScore 0.47
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.461 SNIP 0.709 CiteScore 0.5
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.4 SNIP 0.727 CiteScore 0.44
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.541 SNIP 0.667
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.432 SNIP 0.82
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Dy$_{1-x}$(Gd or Yb)$_x$Ba$_2$Cu$_3$O$_{7-\delta}$ samples were prepared using chemical solution deposition (CSD), based on trifluoroacetate metal-organic decomposition (MOD) methods. X-ray diffraction results demonstrated the formation of the RE123 superconducting phase with a strong in-plane and out-of-plane texture. $c$-lattice constants were observed to decrease for all samples doped with Gd or Yb. Measurements of the onset critical transition temperature ($T^{\text{onset}}$) were found to decrease with increasing Yb content, while only minor changes were observed for samples with Gd. Critical current density ($J_c$) analysis demonstrated that doping with Yb significantly increased the self-field $J_c$ value from 3.8 MA/cm$^2$ to 6.0 MA/cm$^2$ for the pure and 10% Yb doped sample, respectively. In contrast, samples doped with Gd were characterized by the lowest self-field $J_c$ values. Investigation of pinning force mechanisms revealed that the samples in this study were dominated by normal surface pinning.
Synthesis and characterization of 2D layered gadolinium-doped cerium oxide (CGO) nanomaterials

By the virtue of versatility in composition, morphology, and structure, two-dimensional (2D) layered nanomaterials have attracted in the last decade huge interest. Such materials, consisting in stacked charged nanosheets intercalated with opposite charged exchangeable anions, are of great potential for the design and fabrication of nanomaterials in many applications. Indeed, the interlayer gallery provides a flexible space to accommodate various sized molecules (e.g., pollutants) and tune specific active sites at the atomic space (e.g., catalyst materials). The interest for 2D layered nanomaterials is also associated with the possibility of obtaining via exfoliation ultra-thin nanosheets with lateral dimensions of hundreds of nanometres and thickness of few nanometres. This unique class of nanomaterials has shown many unprecedented properties mainly originating from the dimensional anisotropy and nano-confinement effects. Herein we propose novel 2D layered ceria based oxides (e.g., CGO) synthesized via the heterogeneous precipitation. CGO materials were selected because of their strategic relevance in many technological applications (e.g., catalysis and...
electrochemical devices). The synthesized CGO layered materials were characterized for their composition, morphology and crystallographic features. The combined experimental results indicated that the layered CGO, with tunable dopant concentration, can be obtained in different morphologies by controlling the synthesis parameters.

**General information**

State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Instituto de Pesquisas Energeticas e Nucleares, Universidade Federal do ABC
Authors: Poras Reis de Moraes, L. (Ekstern), Marani, D. (Intern), Esposito, V. (Intern), Zanetti De Florio, D. (Ekstern), Coral Fonseca, F. (Ekstern)
Number of pages: 1
Publication date: 2016
Main Research Area: Technical/natural sciences
Electronic versions:
PosterAbstract_dmar.pdf
Source: PublicationPreSubmission
Source-ID: 126278658
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2016

**Synthesis of ligand-free CZTS nanoparticles via a facile hot injection route**

Single-phase, ligand-free Cu2ZnSnS4 (CZTS) nanoparticles that can be dispersed in polar solvents are desirable for thin film solar cell fabrication, since water can be used as the solvent for the nanoparticle ink. In this work, ligand-free nanoparticles were synthesized using a simple hot injection method and the precursor concentration in the reaction medium was tuned to control the final product. The as-synthesized nanoparticles were characterized using various techniques, and were found to have a near-stoichiometric composition and a phase-pure kesterite crystal structure. No secondary phases were detected with Raman spectroscopy or scanning transmission electron microscopy energy dispersive x-ray spectroscopy. Furthermore, high resolution transmission electron microscopy showed large-sized nanoparticles with an average diameter of 23 nm ± 11 nm. This approach avoids all organic materials and toxic solvents that otherwise could hinder grain growth and limit the deposition techniques. In addition the synthesis route presented here results in nanoparticles of a large size compared to other ligand-free CZTS nanoparticles, due to the high boiling point of the solvents selected. Large particle size in CZTS nanoparticle solar cells may lead to a promising device performance. The results obtained demonstrate the suitability of the synthesized nanoparticles for application in low cost thin film solar cells.

**General information**

State: Published
Organisations: Department of Photonics Engineering, Optical Microsensors and Micromaterials, Department of Micro- and Nanotechnology, Silicon Microtechnology, Department of Energy Conversion and Storage, Imaging and Structural Analysis, Department of Physics, Experimental Surface and Nanomaterials Physics, Center for Individual Nanoparticle Functionality, Nanyang Technological University
Authors: Mirbagheri, N. (Intern), Engberg, S. L. J. (Intern), Crovetto, A. (Intern), Simonsen, S. B. (Intern), Hansen, O. (Intern), Lam, Y. M. (Ekstern), Schou, J. (Intern)
Number of pages: 8
Publication date: 2016
Main Research Area: Technical/natural sciences

**Publication information**

Journal: Nanotechnology
Volume: 27
Issue number: 18
ISSN (Print): 0957-4484
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 3.01 SJR 1.079 SNIP 0.788
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.87 SJR 1.339 SNIP 0.945
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.257 SNIP 1.035 CiteScore 3.07
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.497 SNIP 1.269 CiteScore 3.09
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.602 SNIP 1.231 CiteScore 2.74
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.861 SNIP 1.307 CiteScore 3.34
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.899 SNIP 1.451 CiteScore 3.86
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.844 SNIP 1.252
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.809 SNIP 1.27
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.857 SNIP 1.32
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.899 SNIP 1.348
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.938 SNIP 1.364
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.958 SNIP 1.435
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.892 SNIP 1.47
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.475 SNIP 1.364
Web of Science (2003): Indexed yes
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.93 SNIP 0.929
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 0.89 SNIP 0.818
Scopus rating (1999): SJR 0.956 SNIP 0.9
Original language: English
CZTS, Large nanoparticles, Ligand-free, Synthesis
Electronic versions:
Synthesis_of_ligand_free_CZTS_nanoparticles_via_a_facile_hot_injection_route.pdf. Embargo ended: 23/03/2017
DOIs:
10.1088/0957-4484/27/18/185603
Source: FindIt
Source-ID: 277363105
Publication: Research - peer-review › Journal article – Annual report year: 2016

Synthesis of Polybenzimidazoles
General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors, Northeastern University
Authors: Yang, J. (Ekstern), He, R. (Ekstern), Aili, D. (Intern)
Pages: 151-167
Publication date: 2016

Host publication information
Title of host publication: High Temperature Polymer Electrolyte Membrane Fuel Cells: Approaches, Status, and Perspectives
Place of publication: Switzerland
Publisher: Springer
Editors: Li, Q., Aili, D., Hjuler, H. A., Jensen, J. O.
ISBN (Print): 978-3-319-17081-7
ISBN (Electronic): 978-3-319-17082-4
Chapter: 7
Main Research Area: Technical/natural sciences
DOIs: 10.1007/978-3-319-17082-4_7
Publication: Research - peer-review › Book chapter – Annual report year: 2016

Systematic Study of Durability of High Temperature PEM Fuel Cells at Selected Temperatures, Flow Rates and Loads

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors, Danish Power Systems ApS
Authors: Jensen, J. O. (Intern), Jakobsen, M. T. D. (Intern), Cleemann, L. N. (Intern), Steenberg, T. (Ekstern), Hjuler, H. A. (Ekstern), Li, Q. (Intern)
Number of pages: 1
Publication date: 2016
Event: Abstract from PRIME 2016/230th ECS Meeting, Honolulu, United States.
Main Research Area: Technical/natural sciences
Links: https://ecs.confex.com/ecs/230/webprogram/Paper82263.html
Source: PublicationPreSubmission
Source-ID: 127806274
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2016

Techniques for PBI Membrane Characterization

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors, Korea Institute of Science and Technology
Authors: Henkensmeier, D. (Ekstern), Aili, D. (Intern)
Pages: 127-150
Publication date: 2016

Host publication information
Title of host publication: High Temperature Polymer Electrolyte Membrane Fuel Cells: Approaches, Status, and Perspectives
Place of publication: Switzerland
Publisher: Springer
Editors: Li, Q., Aili, D., Hjuler, H. A., Jensen, J. O.
ISBN (Print): 978-3-319-17081-7
ISBN (Electronic): 978-3-319-17082-4
Chapter: 6
Main Research Area: Technical/natural sciences
DOIs: 10.1007/978-3-319-17082-4_6
Publication: Research - peer-review › Book chapter – Annual report year: 2016
Temperature Dependence of Charge Localization in High-Mobility, Solution-Crystallized Small Molecule Semiconductors Studied by Charge Modulation Spectroscopy

In solution-processable small molecule semiconductors, the extent of charge carrier wavefunction localization induced by dynamic disorder can be probed spectroscopically as a function of temperature using charge modulation spectroscopy (CMS). Here, it is shown based on combined field-effect transistor and CMS measurements as a function of temperature that in certain molecular semiconductors, such as solution-processable pentacene, charge carriers become trapped at low temperatures in environments in which the charges become highly localized on individual molecules, while in some other molecules the charge carrier wavefunction can retain a degree of delocalization similar to what is present at room temperature. The experimental approach sheds new insight into the nature of shallow charge traps in these materials and allows identifying molecular systems in which intrinsic transport properties could, in principle, be observed at low temperatures if other transport bottlenecks associated with grain boundaries or contacts could be removed.
The 2016 oxide electronic materials and oxide interfaces roadmap

Oxide electronic materials provide a plethora of possible applications and offer ample opportunity for scientists to probe into some of the exciting and intriguing phenomena exhibited by oxide systems and oxide interfaces. In addition to the already diverse spectrum of properties, the nanoscale form of oxides provides a new dimension of hitherto unknown phenomena due to the increased surface-to-volume ratio. Oxide electronic materials are becoming increasingly important in a wide range of applications including transparent electronics, optoelectronics, magnetoelectronics, photonics, spintronics, thermoelectrics, piezoelectrics, power harvesting, hydrogen storage and environmental waste management. Synthesis and fabrication of these materials, as well as processing into particular device structures to suit a specific application is still a challenge. Further, characterization of these materials to understand the tunability of their properties and the novel properties that evolve due to their nanostructured nature is another facet of the challenge. The research related to the oxide electronic field is at an impressionable stage, and this has motivated us to contribute with a roadmap on 'oxide electronic materials and oxide interfaces'. This roadmap envisages the potential applications of oxide materials in cutting edge technologies and focuses on the necessary advances required to implement these materials, including both conventional and novel techniques for the synthesis, characterization, processing and fabrication of nanostructured oxides and oxide-based devices. The contents of this roadmap will highlight the functional and correlated properties of oxides in bulk, nano, thin film, multilayer and heterostructure forms, as well as the theoretical considerations behind both present and future applications in many technologically important areas as pointed out by Venkatesan. The contributions in this roadmap span several thematic groups which are represented by the following authors: novel field effect transistors and bipolar devices by Fortunato, Grundmann, Boschker, Rao, and Rogers; energy conversion and saving by Zaban, Weidenkaff, and Murakami; new opportunities of photonics by Fompeyrine, and Zuniga-Perez; multiferroic materials including novel phenomena by Ramesh, Spaldin, Mertig, Lorenz, Srinivasan, and Prellier; and concepts for topological oxide electronics by Kawasaki, Pentcheva, and Gegenwart. Finally, Miletto Granozio presents the European action 'towards oxide-based electronics' which develops an oxide electronics roadmap with emphasis on future nonvolatile memories and the required technologies. In summary, we do hope that this oxide roadmap appears as an interesting up-to-date snapshot on one of the most exciting and active areas of solid state physics, materials science, and chemistry, which even after many years of very successful development shows in short intervals novel insights and achievements. Guest editors: M S Ramachandra Rao and Michael Lorenz.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, University of Leipzig, Indian Institute of Technology, Madras, National University of Singapore, Universidade Nova de Lisboa, Qingdao University
Number of pages: 53
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
La$_2$-xCoTiO$_6$-delta/Ce0.9Gd0.1O$_2$-delta composites are presented as promising new cathodes for solid oxide fuel cells. The B-site ordering characteristic of double perovskites is present in the whole series. Additionally, increasing amounts of La-vacancies give rise to ordering of alternating La-rich and square-rich (square = vacancy) Layers perpendicular to the c-axis. The introduction of La vacancies produces both oxidation of Co$^{2+}$ to Co$^{3+}$ and oxygen vacancies inducing a change of both electrical and electrochemical properties. The best electrochemical performances are obtained for Low x due to a compromise between sufficiently high amount of defects to provide electronic and ionic conductivities, but not so high to induce defect clustering. The material with x = 0.05 exhibits the best performances of the series. Symmetrical cells made of composites of this material and Ce0.9Gd0.1O$_2$-delta deposited on pellets of this electrolyte show a polarization resistance of 0.39 Omega cm$^2$ at 1073 K.
The effect of tape casting operational parameters on the quality of adjacently graded ceramic film

For small length tape casting of ceramic slurries varying green film thickness is often a problem. To optimise this, the following parameters were investigated: single blade, double blade, using a pump system and a modelled speed change mode have been analysed. Advantages and limitations of every method are described here. The tape casting experiments were built to be generic in order to allow the control of various processing conditions. From these results, the single-blade technique was chosen for a study of side-by-side tape casting. The influence of the geometric parameters of partitioning the casting tank into chambers, on the quality of graded tape was studied. Tape casting experiments at different speeds and partition tongue lengths in combination with rheological tests revealed that high casting speeds and absence of the partition under the blade are detrimental to the formation of the smooth well-controlled interface between the co-cast slurries, required for most of applications.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Mixed Conductors, Electrofunctional materials
Authors: Bulatova, R. (Intern), Gudik-Sørensen, M. (Intern), Della Negra, M. (Intern), Andersen, K. B. (Intern), Kaiser, A. (Intern), Bahl, C. (Intern)
Number of pages: 9
Pages: 4663-4671
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Ceramics International
Volume: 42
Issue number: 4
ISSN (Print): 0272-8842
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 2.85 SJR 0.784 SNIP 1.167
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.88 SJR 0.844 SNIP 1.376
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.823 SNIP 1.281 CiteScore 2.64
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.856 SNIP 1.645 CiteScore 2.76
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.799 SNIP 1.552 CiteScore 2.28
The Impact of Strong Cathodic Polarization on SOC Electrolyte Materials

One of the most promising reversible energy conversion/storage technologies is that of Solid Oxide Fuel/Electrolysis Cells (SOFC/SOEC, collectively termed SOC). Long term durability is typically required for such devices to become economically feasible, hence considerable amount of work has and is being done on the degradation and long term durability of these systems. When using a SOC in electrolysis mode, it is economically beneficial to operate the cell at high current density, since it increases the fuel production rate. However, several degradation phenomena, such as segregation of impurities at the grain boundaries, electrode poisoning, delamination or cracks of the electrolyte etc., have been observed in cells operated at such conditions, lowering the lifetime of the cell1,2. High polarizations are observed at the electrolyte/cathode interface of an electrolysis cell operated at high current density. In case of a cell voltage above 1.6 V, p-type and n-type electronic conductivity are often observed at the anode and cathode respectively3. Hence, a considerable part of the current is lost as leakage through the electrolyte, thus lowering the efficiency of the cell considerably.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Imaging and Structural Analysis, Department of Chemistry, Fundamental Electrochemistry
Authors: Kreka, K. (Intern), Hansen, K. V. (Intern), Jacobsen, T. (Intern), Norrman, K. (Intern), Chatzichristodoulou, C. (Intern), Mogensen, M. B. (Intern)
Publication date: 2016
The Influence of Conjugated Polymer Side Chain Manipulation on the Efficiency and Stability of Polymer Solar Cells

The stability of polymer solar cells (PSCs) can be influenced by the introduction of particular moieties on the conjugated polymer side chains. In this study, two series of donor-acceptor copolymers, based on bis thiényl dialkoxybenzene donor and benzol[c][1,2,5]thiadiazole (BT) or thiazolo[5,4-d]thiazole (TzTz) acceptor units, were selected toward effective device scalability by roll-coating. The influence of the partial exchange (5% or 10%) of the solubilizing 2-hexyloctoxy by alternative 2-phenylethoxy groups on efficiency and stability was investigated. With an increasing 2-phenylethoxy ratio, a decrease in solar cell efficiency was observed for the BT-based series, whereas the efficiencies for the devices based on the TzTz polymers remained approximately the same. The photochemical degradation rate for PSCs based on the TzTz polymers decreased with an increasing 2-phenylethoxy ratio. Lifetime studies under constant sun irradiance showed a diminishing initial degradation rate for the BT-based devices upon including the alternative side chains, whereas the (more stable) TzTz-based devices degraded at a faster rate from the start of the experiment upon partly exchanging the side chains. No clear trends in the degradation behavior, linked to the copolymer structural changes, could be established at this point, evidencing the complex interplay of events determining PSCs' lifetime.

Conjugated polymers, Side chain variation, Organic photovoltaics, Roll-coating, Photochemical and thermal stability

Electronic versions:
The lifetime cost of a magnetic refrigerator

The total cost of a 25 W average load magnetic refrigerator using commercial grade Gd is calculated using a numerical model. The price of magnetocaloric material, magnet material and cost of operation are considered, and all influence the total cost. The lowest combined total cost with a device lifetime of 15 years is found to be in the range $150-$400 depending on the price of the magnetocaloric and magnet material. The cost of the magnet is largest, followed closely by the cost of operation, while the cost of the magnetocaloric material is almost negligible. For the lowest cost device, the optimal magnetic field is about 1.4 T, the particle size is 0.23 mm, the length of the regenerator is 40-50 mm and the utilization is about 0.2, for all device lifetimes and material and magnet prices, while the operating frequency vary as function of device lifetime. The considered performance characteristics are based on the performance of a conventional A+++ refrigeration unit. In a rough life time cost comparison between the AMR device and such a unit we find similar costs, the AMR being slightly cheaper, assuming the cost of the magnet can be recuperated at end of life.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Authors: Bjørk, R. (Intern), Bahl, C. R. (Intern), Nielsen, K. K. (Intern)
Number of pages: 22
Pages: 48–62
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: International Journal of Refrigeration
Volume: 63
ISSN (Print): 0140-7007
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 1.888 SJR 1.471 CiteScore 3.46
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.06 SJR 1.371 SNIP 1.607
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.349 SNIP 1.532 CiteScore 2.44
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.619 SNIP 2.086 CiteScore 2.6
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.422 SNIP 1.944 CiteScore 2.25
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.386 SNIP 1.893 CiteScore 2.09
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.272 SNIP 2.129 CiteScore 2.2
ISI indexed (2011): ISI indexed yes
The magnetic properties of the hollow cylindrical ideal remanence magnet

We consider the magnetic properties of the hollow cylindrical ideal remanence magnet. This magnet is the cylindrical permanent magnet that generates a uniform field in the cylinder bore, using the least amount of magnetic energy to do so. The remanence distribution of this magnet is derived and the generated field is compared to that of a Halbach cylinder of equal dimensions. The ideal remanence magnet is shown in most cases to generate a significantly lower field than the equivalent Halbach cylinder, although the field is generated with higher efficiency. The most efficient Halbach cylinder is shown to generate a field exactly twice as large as the equivalent ideal remanence magnet.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Authors: Bjørk, R. (Intern)
Number of pages: 4
Pages: 321-324
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Magnetism and Magnetic Materials
Volume: 416
ISSN (Print): 0304-8853
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SJR 0.786 SNIP 1.349 CiteScore 2.97
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Theoretical Insight into the Trends that Guide the Electrochemical Reduction of Carbon Dioxide to Formic Acid

The electrochemical reduction (electroreduction) of CO$_2$ to formic acid (HCOOH) and its competing reactions, that is, the electroreduction of CO$_2$ to CO and the hydrogen evolution reaction (HER), on twenty-seven different metal surfaces have been investigated using density functional theory (DFT) calculations. Owing to a strong linear correlation between the free energies of COOH$^*$ and H$^*$, it seems highly unlikely that the electroreduction of CO$_2$ to HCOOH via the COOH$^*$ intermediate occurs without a large fraction of the current going to HER. On the other hand, the selective electroreduction of CO$_2$ to HCOOH seems plausible if the reaction occurs via the HCOO$^*$ intermediate, as there is little correlation between the free energies of HCOO$^*$ and H$^*$. Lead and silver surfaces are found to be the most promising monometallic catalysts showing high faradaic efficiencies for the electroreduction of CO$_2$ to HCOOH with small overpotentials. Our methodology is widely applicable, not only to metal surfaces, but also to other classes of materials enabling the computational search for electrocatalysts for CO$_2$ reduction to HCOOH.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, Stanford University, SLAC National Accelerator Laboratory
Authors: Yoo, J. (Ekstern), Christensen, R. (Intern), Vegge, T. (Intern), Nørskov, J. (Ekstern), Studt, F. (Ekstern)
Number of pages: 7
Pages: 358 – 363
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: ChemSusChem (Print)
Volume: 9
ISSN (Print): 1864-5631
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 6.86 SJR 2.538 SNIP 1.235
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 6.7 SJR 2.505 SNIP 1.311
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 2.53 SNIP 1.424 CiteScore 7.33
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.864 SNIP 1.663 CiteScore 7.97
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 2.561 SNIP 1.46 CiteScore 6.79
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Scopus rating (2012): SJR 3.054 SNIP 1.553 CiteScore 6.72
ISI indexed (2012): ISI indexed yes
Scopus rating (2011): SJR 2.759 SNIP 1.497 CiteScore 5.53
ISI indexed (2011): ISI indexed no
Web of Science (2011): Indexed yes
Scopus rating (2010): SJR 1.959 SNIP 1.143
Web of Science (2010): Indexed yes
Scopus rating (2009): SJR 0.979 SNIP 0.718
BFI (2008): BFI-level 1
Theoretical Limiting Potentials in Mg/O2 Batteries

A rechargeable battery based on a multivalent Mg/O2 couple is an attractive chemistry due to its high theoretical energy density and potential for low cost. Nevertheless, metal-air batteries based on alkaline earth anodes have received limited attention and generally exhibit modest performance. In addition, many fundamental aspects of this system remain poorly understood, such as the reaction mechanisms associated with discharge and charging. The present study aims to close this knowledge gap and thereby accelerate the development of Mg/O2 batteries by employing first-principles calculations to characterize electrochemical processes on the surfaces of likely discharge products, MgO and MgO2. Thermodynamic limiting potentials for charge and discharge are calculated for several scenarios, including variations in surface stoichiometry and the presence/absence of intermediate species in the reaction pathway. The calculations indicate that pathways involving oxygen intermediates are preferred, as they generally result in higher discharge and lower charging voltages. In agreement with recent experiments, cells that discharge to MgO exhibit low round-trip efficiencies, which are rationalized by the presence of large thermodynamic overvoltages. In contrast, MgO2-based cells are predicted to be much more efficient: superoxide-terminated facets on MgO2 crystallites enable low overvoltages and round-trip efficiencies approaching 90%. These data suggest that the performance of Mg/O2 batteries can be dramatically improved by biasing discharge toward the formation of MgO2 rather than MgO.
The Organic Power Transistor: Roll-to-Roll Manufacture, Thermal Behavior, and Power Handling When Driving Printed Electronics

We present flexible organic power transistors prepared by fast (20min1) roll-to-roll (R2R) flexographic printing[1] of the drain (D) and source (S) electrode structures directly on polyester foil. The devices have top gate architecture and were completed by spin coating or slot-die coating of the organic semiconductor poly-3-hexylthiophene (P3HT) and the dielectric material polyvinylphenol (PVP) before the gate (G) was applied by either screen printing or evaporation of silver.
We explore the footprint and the practically accessible geometry of such devices with a special view toward being able to drive large currents while handling the thermal aspects in operation together with other organic printed electronics technologies such as large area organic photovoltaics (OPV)[2] and large area electrochromic displays (EC).[3] We find especially that an elevated operational temperature is beneficial with respect to both transconductance and on/off ratio. We achieve high currents of up to 45mA at a temperature of 80 C with an on/off ratio of 100 which is sufficient to drive large area organic electronics such as an EC device powered by OPV devices that we also demonstrate. Finally, we observe a significant temperature dependence of the performance which can be explored further in sensing applications.
Thermal analysis of CZTS nanoparticles and inks

General information
State: Published
Organisations: Department of Photonics Engineering, Department of Energy Conversion and Storage, Mixed Conductors, Department of Micro- and Nanotechnology, Silicon Microtechnology, Experimental Surface and Nanomaterials Physics, Optical Microsensors and Micromaterials, Nanyang Technological University
Authors: Engberg, S. L. J. (Intern), Agersted, K. (Ekstern), Crovetto, A. (Intern), Hansen, O. (Intern), Lam, Y. M. (Ekstern), Schou, J. (Intern)
Publication date: 2016
Event: Poster session presented at 2016 E-MRS Spring Meeting and Exhibit, Lille, France.
Main Research Area: Technical/natural sciences
Publication: Research - peer-review › Journal article – Annual report year: 2015

Thermal decomposition of heavy rare-earth butanoates, \(\text{Ln}(C_3H_7CO_2)_3\) (\(\text{Ln} = \text{Er, Tm, Yb and Lu}\)) in argon

The thermal behaviour of \(\text{Ln}(C_3H_7CO_2)_3\) (\(\text{Ln} = \text{Er, Tm, Yb or Lu}\)) was studied in argon from room temperature by means of thermogravimetry and differential thermal analysis up to 1400 °C, by infrared spectroscopy, hot-stage optical microscopy and X-ray diffraction. Melting prior to decomposition was observed in all four compounds, but its course depends on the rare-earth element. Decomposition to sesquioxides proceeds via the formation of dioxymonocarbonates (\(\text{Ln}_2\text{O}_2\text{CO}_3\)) and release of 4-heptanone (\(C_3H_7COC_3H_7\)) as well as carbon dioxide (\(\text{CO}_2\)) without evidence for an intermediate oxobutanoate stage. During the decomposition of \(\text{Ln}_2\text{O}_2\text{CO}_3\) into the respective sesquioxides (\(\text{Ln}_2\text{O}_3\)), an intermediate plateau extending from approximately 550 to 850 °C appears in the TG traces. The overall composition during this stage corresponds approximately to \(\text{Ln}_2\text{O}_{2.8}\text{CO}_3\), but the state is more probably a mixture of \(\text{Ln}_2\text{O}_2\text{CO}_3\) and \(\text{Ln}_2\text{O}_3\). The stability of this intermediate state seems to decrease with the mass of the rare-earth elements. Complete conversion to \(\text{Ln}_2\text{O}_3\) is reached at about 1100 °C. The overall thermal decomposition behaviour of the title compounds is different from previous reports for other rare-earth butanoates.
Thermal decomposition of Yttrium(III) isovalerate in argon

The thermal behaviour of yttrium(III) isovalerate (Y(C₄H₉CO₂)₃) was studied in argon by means of thermogravimetry, differential thermal analysis, FTIR-spectroscopy, hot-stage optical microscopy and X-ray diffraction with a laboratory Cu-tube source as well as with a synchrotron radiation source. Two structural transitions take place in the solid state at 100 ºC and 140 ºC. They are followed by the decomposition of the isovalerate salt with release of gaseous products consisting of CO₂ and 2,6-dimethyl-4-heptanone and formation of Y₂O₂CO₃ between 320 ºC and 440 ºC. Above 440 ºC, Y₂O₂CO₃ is
slowly converted to $\text{Y}_2\text{O}_3$ with release of $\text{CO}_2$. The decomposition is complete at about 900 °C.

**General information**

State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Deutsches Elektronen-Synchrotron
Authors: Grivel, J. (Intern), Yue, Z. (Intern), Tang, X. (Intern), Pallewatta, P. G. A. P. (Intern), Watenphul, A. (Ekstern), von Zimmermann, M. (Ekstern)
Number of pages: 6
Pages: 341-346
Publication date: 2016
Main Research Area: Technical/natural sciences

**Publication information**

Journal: Journal of Analytical and Applied Pyrolysis
Volume: 120
ISSN (Print): 0165-2370
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 1.312 SJR 1.129 CiteScore 3.91
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.11 SJR 1.379 SNIP 1.572
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.489 SNIP 1.635 CiteScore 4.06
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.691 SNIP 1.954 CiteScore 4.08
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.036 SNIP 1.921 CiteScore 3.6
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.408 SNIP 1.77 CiteScore 3.26
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.388 SNIP 1.603 CiteScore 3.07
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.181 SNIP 1.424
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.296 SNIP 1.418
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.247 SNIP 1.43
Scopus rating (2007): SJR 1.334 SNIP 1.977
Scopus rating (2006): SJR 0.87 SNIP 1.408
Scopus rating (2005): SJR 0.792 SNIP 1.238
Scopus rating (2004): SJR 1.086 SNIP 1.242
Scopus rating (2003): SJR 0.607 SNIP 1.353
Scopus rating (2002): SJR 1.59 SNIP 1.229
Scopus rating (2001): SJR 1.254 SNIP 1.506
Web of Science (2001): Indexed yes
Thermo-Chemo-Mechanical Response of Solid Oxide Cells during Reduction and Cooling

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Imaging and Structural Analysis, Atomic scale modelling and materials, Amminex Emissions Technology A/S
Authors: Chatzichristodoulou, C. (Intern), Charlas, B. (Ekstern), Kwok, K. (Intern), Jørgensen, P. S. (Intern), Norby, P. (Intern), Hendriksen, P. V. (Intern), Frandsen, H. L. (Intern)
Number of pages: 1
Publication date: 2016
Conference: The 229th ECS Meeting, San Diego, CA, United States, 29/05/2016 - 29/05/2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Electrochemical Society. Meeting Abstracts (Online)
Volume: MA2016-01
Article number: 1495
ISSN (Print): 2151-2043
Original language: English
Electronic versions:
Thermo_Chemo_Mechanical.pdf
Links:
http://ma.ecsdl.org/content/MA2016-01/30/1495.abstract
Source: PublicationPreSubmission
Source-ID: 128053340
Publication: Research - peer-review › Conference abstract in journal – Annual report year: 2016

Thermodynamic modeling of the Sr-Co-Fe-O system
This paper reviews and assesses phase equilibria and thermodynamic properties of phases in the Sr-Co-Fe-O system, with a focus on oxides, especially the SrCo$_{1-x}$Fe$_x$O$_{3-\delta}$ perovskite. In our work, the SrCo$_{1-x}$Fe$_x$O$_{3-\delta}$ perovskite was modeled with a three-sublattice model, where the three sublattices correspond to the A, B and oxygen sites in an ABO$_3$ perovskite, respectively. A number of other important ternary oxide phases in Sr-Co-O and Sr-Co-Fe-O were also considered. Available thermodynamic and phase diagram data were carefully assessed. A thermodynamic description of Sr-Co-O was derived using the CALPHAD approach and was further extrapolated to that of Sr-Co-Fe-O. The thermodynamic database of Sr-Co-Fe-O established in this work allows for calculating phase diagrams, thermodynamic properties, cation distribution and defect chemistry properties, and therefore enables material composition optimization for various applications, including solid oxide fuel cells and oxygen membranes.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Imaging and Structural Analysis, Mixed Conductors, Vienna University of Technology
Authors: Zhang, W. W. (Intern), Povoden-Karadeniz, E. (Ekstern), Chen, M. (Intern), Hendriksen, P. V. (Intern)
Number of pages: 10
Pages: 88-97
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Solid State Ionics
Volume: 282
ISSN (Print): 0167-2738
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 2.64 SJR 0.856 SNIP 0.952
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.41 SJR 0.75 SNIP 0.909
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.802 SNIP 1.016 CiteScore 2.5
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.837 SNIP 1.282 CiteScore 2.62
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.903 SNIP 1.269 CiteScore 2.35
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.051 SNIP 1.253 CiteScore 2.31
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.376 SNIP 1.615 CiteScore 2.96
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.46 SNIP 1.498
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.508 SNIP 1.483
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.515 SNIP 1.617
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.292 SNIP 1.384
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.239 SNIP 1.541
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.093 SNIP 1.423
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.18 SNIP 1.55
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.473 SNIP 1.389
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 1.253 SNIP 1.36
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 1.121 SNIP 1.213
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 1.161 SNIP 1.312
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 1.08 SNIP 1.254

Original language: English
Thermoelectric Properties of Solution-Processed n-Doped Ladder-Type Conducting Polymers

Ladder-type "torsion-free" conducting polymers (e.g., polybenzimidazobenzophenanthroline (BBL)) can outperform "structurally distorted" donor-acceptor polymers (e.g., P(NDI2OD-T2)), in terms of conductivity and thermoelectric power factor. The polaron delocalization length is larger in BBL than in P(NDI2OD-T2), resulting in a higher measured polaron mobility. Structure-function relationships are drawn, setting material-design guidelines for the next generation of conducting thermoelectric polymers.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Imaging and Structural Analysis, Linköping University, Max-Planck-Institut fur Kohlenforschung
Number of pages: 8
Pages: 10764–10771
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Advanced Materials
Volume: 28
Issue number: 48
ISSN (Print): 0935-9648
Ratings:
BFI (2018): BFI-level 3
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 21.1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 17.79
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 18.5
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 16.79
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 15.78
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 14.41
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 12.28
ISI indexed (2011): ISI indexed yes
This paper presents a constitutive thermoviscoelastic model for thin films of linear low-density polyethylene subject to strains up to yielding. The model is based on the free volume theory of nonlinear thermoviscoelasticity, extended to orthotropic membranes. An ingredient of the present approach is that the experimentally inaccessible out-of-plane material properties are determined by fitting the model predictions to the measured nonlinear behavior of the film. Creep tests, uniaxial tension tests, and biaxial bubble tests are used to determine the material parameters. The model has been validated experimentally, against data obtained from uniaxial tension tests and biaxial cylindrical tests at a wide range of temperatures and strain rates spanning two orders of magnitude.
Nonlinear viscoelasticity, Free volume model, Polymer thin film

DoIs:
10.1007/s11043-015-9282-8

The role of hydrogen bonds in the melting points of sulfonate-based protic organic salts

There are three main types of interactions inside organic salts - electrostatic interaction, hydrogen bonding and van der Waals force [1-4]. While van der Waals force is relatively weak, it is hydrogen bonding and particularly electrostatic interaction that determine the lattice energies of ionic systems and other physicochemical properties like melting points [5]. The hydrogen bond is an attractive interaction between a hydrogen atom from a molecule or a molecular fragment X-H in which X is more electronegative than H, and an atom or a group of atoms in the same or a different molecule, in which there is evidence of bond formation [6]. Hydrogen bonds in the solid state fall into the classification of strong, moderate, and weak hydrogen bonds [7]. In molecular systems like H₂O (vs. H₂S) or NH₃ (vs. PH₃), strong hydrogen bonds lead to higher melting points. However, in organic salts, the situation may be different [8,9].

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Technical University of Denmark
Authors: Luo, J. (Ekstern)
Pages: 177-177
Publication date: 2016

Host publication information
Title of host publication: ISPE-XV, Uppsala 15-19th August 2016
Article number: P52
Main Research Area: Technical/natural sciences
Electronic versions:
The_role_of_hydrogen_bonds_in_the_melting_points_of_sulfonate_based_protic.pdf
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2016
Thin films for energy conversion and storage devices: status and perspective

General information
State: Published
Organisations: Fundamental Electrochemistry, Department of Energy Conversion and Storage
Authors: Stamate, E. (Intern)
Number of pages: 1
Publication date: 2016
Main Research Area: Technical/natural sciences
Electronic versions:
Thin_films_for_energy.pdf

Bibliographical note
Invited lecture
Source: PublicationPreSubmission
Source-ID: 128141809
Publication: Research › Conference abstract for conference – Annual report year: 2016

Three-dimensional numerical modeling of an induction heated injection molding tool with flow visualization

Using elevated mold temperature is known to have a positive influence of final injection molded parts. Induction heating is a method that allow obtaining a rapid thermal cycle, so the overall molding cycle time is not increased. In the present research work, an integrated multi-turn induction heating coil has been developed and assembled into an injection molding tool provided with a glass window, so the effect of induction heating can directly be captured by a high speed camera. In addition, thermocouples and pressure sensors are also installed, and together with the high speed videos, comparison of the induction heating and filling of the cavity is compared and validated with simulations. Two polymer materials ABS and HVPC were utilized during the injection molding experiments carried out in this work. A nonlinear electromagnetic model was employed to establish an effective linear magnetic permeability. The three-dimensional transient thermal field of the mold cavity was then calculated and compared with the experiments. This thermal field was transferred to an injection molding flow solver to compare simulations and experimental results from the high speed video, both with and without the effect of induction heating. A rapid thermal cycle was proved to be feasible in a mold with an integrated induction coil. Furthermore, it was shown that the process can be modeled with good accuracy, both in terms of the thermal field and of the flow pattern.

General information
State: Published
Organisations: Department of Mechanical Engineering, Manufacturing Engineering, Department of Energy Conversion and Storage, Electrofunctional materials
Authors: Guerrier, P. (Intern), Tosello, G. (Intern), Nielsen, K. K. (Intern), Hattel, J. H. (Intern)
Number of pages: 18
Pages: 643-660
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: International Journal of Advanced Manufacturing Technology
Volume: 85
Issue number: 1
ISSN (Print): 0268-3768
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 2.8 SJR 0.994 SNIP 1.697
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.3 SJR 1.046 SNIP 1.608
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.889 SNIP 1.325 CiteScore 1.8
Tracking Electronic Pathways in Energy Materials by Low Voltage Scanning Electron Microscopy

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Imaging and Structural Analysis
Authors: Bentzen, J. J. (Intern), Thydén, K. T. S. (Intern)
Number of pages: 1
Publication date: 2016
Event: Poster session presented at SCANDEM 2016, Trondheim, Norway.
Tracking Electronic Pathways in Energy Materials by Low Voltage Scanning Electron Microscopy

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Imaging and Structural Analysis
Authors: Bentzen, J. J. (Intern), Thydén, K. T. S. (Intern)
Number of pages: 1
Publication date: 2016
Main Research Area: Technical/natural sciences
electronic pathways, surface potential contrast, low voltage SEM, solid oxide cells, energy materials
Electronic versions:
SCANDEM2016_poster_abstract_jabe_thyd_4.pdf
Source: PublicationPreSubmission
Source-ID: 124915494
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2016

Transparent and low emissivity coatings based on aluminum doped zinc oxide

General information
State: Published
Organisations: Fundamental Electrochemistry, Department of Energy Conversion and Storage
Authors: Stamate, E. (Intern)
Number of pages: 1
Publication date: 2016
Event: Abstract from 4th International Workshop on Solution Plasma and Molecular Technologies, Pilsen, Czech Republic.
Main Research Area: Technical/natural sciences
Electronic versions:
Transparent_and_low_emissivity.pdf
Source: PublicationPreSubmission
Source-ID: 128141847
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2016

Tubular asymmetric oxygen transport membranes

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Mixed Conductors
Authors: Bjørnetun Haugen, A. (Intern), Ovtar, S. (Intern), Gurauskis, J. (Intern), Kaiser, A. (Intern), Hendriksen, P. V. (Intern)
Number of pages: 1
Publication date: 2016
Event: Abstract from 6th International Conference on Shaping of Advanced Ceramics, Montpellier, France.
Main Research Area: Technical/natural sciences
Electronic versions:
Tubular_asymmetric_oxygen.pdf

Bibliographical note
Oral presentation
Source: PublicationPreSubmission
Source-ID: 127726185
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2016

Tuning the activity of Pt alloy electrocatalysts by means of the lanthanide contraction
The high platinum loadings required to compensate for the slow kinetics of the oxygen reduction reaction (ORR) impede the widespread uptake of low-temperature fuel cells in automotive vehicles. We have studied the ORR on eight platinum
lanthanide and Pt-alkaline earth electrodes, Pt5M, where M is lanthanum, cerium, samarium, gadolinium, terbium, dysprosium, thulium, or calcium. The materials are among the most active polycrystalline Pt-based catalysts reported, presenting activity enhancement by a factor of 3 to 6 over Pt. The active phase consists of a Pt overlayer formed by acid leaching. The ORR activity versus the bulk lattice parameter follows a high peaked “volcano” relation. We demonstrate how the lanthanide contraction can be used to control strain effects and tune the activity, stability, and reactivity of these materials.

General information
State: Published
Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics, Center for Individual Nanoparticle Functionality, Center for Atomic-scale Materials Design, Theoretical Atomic-scale Physics, Department of Energy Conversion and Storage, Atomic scale modelling and materials
Number of pages: 4
Pages: 73-76
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Science
Volume: 352
Issue number: 6281
ISSN (Print): 0036-8075
Ratings:
BFI (2018): BFI-level 3
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 15.85 SJR 14.142 SNIP 7.154
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 14.39 SJR 13.745 SNIP 7.547
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 12.052 SNIP 8.129 CiteScore 12.68
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 12.41 SNIP 7.809 CiteScore 12.43
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 14.238 SNIP 8.277 CiteScore 11.97
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 13.481 SNIP 7.773
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 11.897 SNIP 7.056
Web of Science (2009): Indexed yes
Understanding degradation of solid oxide electrolysis cells through modeling of electrochemical potential profiles
Establishing the spatial distribution of the various chemical and electrochemical potentials in an operating SOEC is critical as several degradation mechanisms are tightly connected to them, but at the same time very challenging to achieve experimentally. Such distributions are presented here on the basis of a two dimensional bi-layer electrolyte SOC model including for both electrodes a description of activation, concentration, and conversion losses. An extensive parametric study is reported to illustrate the influence of the electrode polarization resistances, the ionic and electronic conductivities in the electrolyte, the gas composition, temperature, and pressure on the current density distribution over the cell and the oxygen activity distribution within the electrolyte. The developed model is further used to simulate long-term durability experiments during different stages of operation, thereby helping to rationalize microstructural and chemical changes observed in post-mortem analysis. Finally, measures to mitigate degradation by changing conditions of operation, material or electrode properties or overall cell geometry are suggested.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Fundamental Electrochemistry, Mixed Conductors, Department of Chemistry
Authors: Chatzichristodoulou, C. (Intern), Chen, M. (Intern), Hendriksen, P. V. (Intern), Jacobsen, T. (Intern), Mogensen, M. B. (Intern)
Number of pages: 18
Pages: 265-282
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Electrochimica Acta
Volume: 189
ISSN (Print): 0013-4686
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
bi-layer electrolyte, degradation, electrochemical potential profiles, modeling, SOEC

DOIs:
10.1016/j.electacta.2015.12.067

Original language: English

bi-layer electrolyte, degradation, electrochemical potential profiles, modeling, SOEC

DOIs:
10.1016/j.electacta.2015.12.067

Source: FindIt
Source-ID: 2289880746
Publication: Research - peer-review › Journal article – Annual report year: 2016
**Understanding ternary poly(potassium benzimidazolide)-based polymer electrolytes**

Poly(2,20-(m-phenylene)-5,50-bisbenzimidazole) (m-PBI) can dissolve large amounts of aqueous electrolytes to give materials with extraordinary high ion conductivity and the practical applicability has been demonstrated repeatedly in fuel cells, water electrolyzers and as anion conducting component in fuel cell catalyst layers. This work focuses on the chemistry of m-PBI in aqueous potassium hydroxide. Equilibration in aqueous KOH with concentrations of 15e20 wt.% was found to result in ionization of the polymer, causing released intermolecular hydrogen bonding. This allowed for extensive volume swelling, high electrolyte uptake, dramatic plasticization and increase of the ion conductivity for the formed poly(potassium benzimidazolide)-based structure. Further increasing the concentration of the bulk solution to 50 wt.% resulted in dehydration and extensive crystallization of the polymer matrix as evidenced by X-ray diffraction, increased density and enhanced elastic modulus. © 2016 Elsevier Ltd. All rights reserved.
Understanding the Thermodynamic Properties of the Elastocaloric Effect Through Experimentation and Modelling

This paper presents direct and indirect methods for studying the elastocaloric effect (eCE) in shape memory materials and its comparison. The eCE can be characterized by the adiabatic temperature change or the isothermal entropy change (both as a function of applied stress/strain). To get these quantities, the evaluation of the eCE can be done using either direct methods, where one measures (adiabatic) temperature changes or indirect methods where one can measure the stress–strain–temperature characteristics of the materials and from these deduce the adiabatic temperature and isothermal entropy changes. The former can be done using the basic thermodynamic relations, i.e. Maxwell relation and Clausius–Clapeyron equation. This paper further presents basic thermodynamic properties of shape memory materials, such as the adiabatic temperature change, isothermal entropy change and total entropy–temperature diagrams (all as a function of temperature and applied stress/strain) of two groups of materials (Ni–Ti and Cu–Zn–Al alloys) obtained using indirect methods through phenomenological modelling and Maxwell relation. In the last part of the paper, the basic definition of the efficiency of the elastocaloric thermodynamic cycle (coefficient of performance) is defined and discussed.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, University of Ljubljana, Universitat de Barcelona
Authors: Tušek, J. (Ekstern), Engelbrecht, K. (Intern), Mañosa, L. (Ekstern), Vives, E. (Ekstern), Pryds, N. (Intern)
Pages: 317-329
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Shape Memory and Superelasticity
Volume: 2
Issue number: 4
ISSN (Print): 2199-384X
Original language: English
Universality in Nonaqueous Alkali Oxygen Reduction on Metal Surfaces: Implications for Li−O2 and Na−O2 Batteries
Nonaqueous metal−oxygen batteries, particularly lithium−oxygen and sodium−oxygen, have emerged as possible high energy density alternatives to Li-ion batteries that could address the limited driving range issues faced by electric vehicles. Many fundamental questions remain unanswered, including the origin of the differences in the discharge product formed, i.e., Li2O2 versus Li2O in Li−O2 batteries and NaO2 versus Na2O2 in Na−O2 batteries. In this Letter, we analyze the role of the electrode (electrocatalyst) in determining the selectivity of the discharge product through a tuning of the nucleation overpotential for a given electrolyte. On the basis of a thermodynamic analysis using density functional theory calculations, we demonstrate that the free energy of adsorbed LiO2* is a descriptor determining the nucleation overpotential for the formation of lithium peroxide, Li2O2, the primary discharge product in Li−O2 batteries. Our analysis suggests that Au(100), Ag(111), and Au(111) are capable of nucleating Li2O2 with very low overpotentials. We also show that the free energy of adsorbed NaO2* is a descriptor determining the nucleation rate for sodium superoxide, NaO2, the primary discharge product in Na−O2 batteries. We explore trends in selectivity between 2e− and 4e− oxygen reduction for nucleating Li2O2 and Li2O, respectively, and show that to a first approximation, the selectivity can be determined by a single descriptor, the free energy of adsorbed LiO2*. This is due to the existence of linear scaling between LiO2* and LiO* similar to that observed for OOH* and OH* for aqueous oxygen reduction. This analysis shows that for all materials that possess low nucleation overpotentials, the nucleation overpotential for 2e− oxygen reduction is smaller than that for the 4e− oxygen reduction. In the case of Na−O2, we find that the trends in selectivity between nucleating NaO2 and Na2O2 are determined by the free energy of adsorbed NaO2* and the reorganization energy associated with sodium-ion coupled electron transfer. This analysis provides a rational basis for the selection of the electrode (electrocatalyst) for tuning the nucleation and thereby potentially controlling the discharge product.

Voltage and Thermally Driven High Current RolltoRoll Printed Transistors
General information
State: Published
Organisations: Department of Energy Conversion and Storage, Organic Energy Materials
Authors: Pastorelli, F. (Intern)
Number of pages: 1
Publication date: 2016
Event: Abstract from 2016 MRS Fall Meeting & Exhibit, Boston, MA, United States.
Main Research Area: Technical/natural sciences
Water vapor pressure over molten KH$_2$PO$_4$ and demonstration of water electrolysis at ∼300°C

A new potentially high-efficiency electrolyte for water electrolysis: molten monobasic potassium phosphate, KH$_2$PO$_4$ or KDP has been investigated at temperatures ∼275–325 °C. At these temperatures, KH$_2$PO$_4$ was found to dissociate into H$_2$O gas in equilibrium with a melt mixture of KH$_2$PO$_4$–K$_2$H$_2$P$_2$O$_7$–KPO$_3$–H$_2$O. The water vapor pressure above the melt, when contained in a closed ampoule, was determined quantitatively vs. temperature by use of Raman spectroscopy with methane or hydrogen gas as an internal calibration standard, using newly established relative ratios of Raman scattering cross sections of water and methane or hydrogen to be 0.40 ± 0.02 or 1.2 ± 0.03. At equilibrium the vapor pressure was much lower than the vapor pressure above liquid water at the same temperature. Electrolysis was realized by passing current through closed ampoules (vacuum sealed quartz glass electrolysis cells with platinum electrodes and the electrolyte melt). The formation of mixtures of hydrogen and oxygen gases as well as the water vapor was detected by Raman spectroscopy. In this way it was demonstrated that water is present in the new electrolyte: molten KH$_2$PO$_4$ can be split by electrolysis via the reaction 2H$_2$O → 2H$_2$ + O$_2$ at temperatures ∼275–325 °C. At these temperatures, before the start of the electrolysis, the KH$_2$PO$_4$ melt gives off H$_2$O gas that pressurizes the cell according to the following dissociations: 2KH$_2$PO$_4$ ↔ K$_2$H$_2$P$_2$O$_7$ + H$_2$O ↔ 2KPO$_3$ + 2H$_2$O. The spectra show however that the water by virtue of hydrogen-bonding has a high affinity for remaining in the melt. The formed hydrogen and oxygen gasses were detected by means of the characteristic Raman gas-phase spectra.
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.416 SNIP 2.827 CiteScore 5.5
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.531 SNIP 2.259
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.992 SNIP 1.85
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 0.95 SNIP 1.206
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.168 SNIP 1.704
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 0.95 SNIP 1.277
Scopus rating (2005): SJR 1.02 SNIP 0.988
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.67 SNIP 0.844
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 0.713 SNIP 0.775
Scopus rating (2002): SJR 0.589 SNIP 0.779
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.368 SNIP 0.567
Scopus rating (2000): SJR 0.154 SNIP 0.498
Scopus rating (1999): SJR 0.181 SNIP 0.443
Original language: English
Molten salt electrolyte, KDP, Elevated temperature water electrolysis, Vapor pressure, Phosphate-based electrolytes, Raman spectroscopy, Water electrolysis
Electronic versions:
Water_vapor_pressure_over_molten_KH2PO4_and_demonstration_of_water_electrolysis_at_300_C.postprint.pdf. Embargo ended: 28/07/2018
294_Water_vapor_pressure_over_molten_KH2PO4_2016_07_15_resubmitted.pdf. Embargo ended: 04/08/2018
DOIs:
10.1016/j.apenergy.2016.07.123
Publication: Research - peer-review › Journal article – Annual report year: 2016

Which Electrode Materials to Select for More Environmentally Friendly Organic Photovoltaics?

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Functional organic materials, Department of Management Engineering, Quantitative Sustainability Assessment
Authors: Espinosa Martinez, N. (Intern), Laurent, A. (Intern), Benatto, G. A. D. R. (Intern), Hösel, M. (Intern), Krebs, F. C. (Intern)
Number of pages: 6
Pages: 490-495
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Advanced Engineering Materials
Volume: 18
Issue number: 4
ISSN (Print): 1438-1656
Ratings:
BFI (2018): BFI-level 1
**Zero carbon energy system of South East Europe in 2050**

South East Europe is the region in a part of Europe with approximately 65.5 million inhabitants, making up 8.9% of Europe's total population. The countries concerned have distinct geographical features, various climates and significant differences in gross domestic product per capita, so the integration of their energy systems is considered to be a challenging task. Large differences between energy mixes, still largely dominated by fossil-fuel consumption, make this task even more demanding. This paper presents the transition steps to a 100% renewable energy system which need to be carried out until the year 2050 in order to achieve zero carbon energy society. Novelty of this paper compared to other papers with similar research goals is the assumed sustainable use of biomass in the 100% renewable energy system of the region considered. It is important to emphasize here that only the sustainable use of biomass can be considered carbon-neutral. The resulting biomass consumption of the model was 725.94 PJ for the entire region, which is in line with the biomass potential of the region. Modelling the zero-carbon energy system was carried out using the smart energy system concept, together with its main integration pillars, i.e., power-to-heat and power-to-gas technologies. The resulting power generation mix shows that a wide variety of energy sources need to be utilized and no single energy source has more than a 30% share, which also increases the security of supply. Wind turbines and photovoltaics are the main technologies with shares of 28.9% and 22.5%, followed by hydro power, concentrated solar power, biomass (mainly used in cogeneration units) and geothermal energy sources. To keep the biomass consumption within the sustainability limits, there is a need for some type of synthetic fuel in the transportation sector. Nevertheless, achieving 100% renewable energy system also promises to be financially beneficial, as the total calculated annual socio-economic cost of the region is approximately 20 billion euros lower in the year 2050 than in the base year. Finally, energy efficiency measures will play an important role in the transition to the zero-carbon energy society: the model shows that primary energy supply will be 50.9% lower than in the base year.

**General information**

State: Published

Organisations: Department of Energy Conversion and Storage, University of Zagreb, International Centre for Sustainable Development of Energy, Water and Environment Systems

Authors: Dominkovic, D. F. (Intern), Bačeković, I. (Ekstern), Ćosić, B. (Ekstern), Krajačić, G. (Ekstern), Pukšec, T. (Ekstern), Duč, N. (Ekstern), Markovska, N. (Ekstern)

Number of pages: 12
Zero carbon energy system of south east europe in 2050 - poster

South East Europe consists of several smaller countries in terms of energy systems and thus, integrating energy systems of the whole region has significant benefits for all the countries included. However, as there are large differences between energy mixes of the countries included, careful energy planning needs to be carried out in order to satisfy energy needs of all the countries of the region. Due to the significant differences in geography and the climate of different parts of the region, many different technologies need to be introduced in order to have optimal, low-carbon energy mix. In this paper, steps toward the 100% renewable energy system (RES) for the year 2050 have been presented. Novelty in this paper, compared to the similar research already being carried out, is the sustainable use of biomass in 100% RES, as this is the only way in which biomass can be considered as carbon-neutral. Smart energy systems’ approach has been used in planning of 100% RES, which considers significant integration of the electrical, heating and gas sectors. Many technologies have been employed in the year 2050, but the major share is put on photovoltaics and wind energy, followed by geothermal, solar thermal, CHPs driven on biomass, hydro power and synthetic fuel technologies. Finally, it was shown that the 100% RES in the year 2050 is cheaper than the reference system, developed for the year 2012.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Centre for IT-Intelligent Energy Systems in Cities, Aalborg University, University of Zagreb, Macedonian Academy of Arts and Science
Authors: Dominkovic, D. F. (Intern), Bačeković, I. (Ekstern), Ćosić, B. (Ekstern), Krajačić, G. (Ekstern), Pukšec, T. (Ekstern), Duć, N. (Ekstern), Markovska, N. (Ekstern)
Number of pages: 1
Publication date: 2016
Event:
Main Research Area: Technical/natural sciences
Electronic versions:
Zero_carbon_energy_system_of_south_east_europe_in_2050_poster.pdf
Source: PublicationPreSubmission
Source-ID: 125442958
Publication: Research - peer-review › Poster – Annual report year: 2016

Zero-Gap Alkaline Water Electrolysis Using Ion-Solvating Polymer Electrolyte Membranes at Reduced KOH Concentrations

Membranes based on poly(2,2’-(m-phenylene)-5,5-bibenzimidazole) (m-PBI) can dissolve large amounts of aqueous KOH to give electrolyte systems with ion conductivity in a practically useful range. The conductivity of the membrane strongly depends on the concentration of the aqueous KOH phase, reaching about 10^{-1} S cm^{-1} or higher in 15-25 wt% KOH. Herein, m-PBI membranes are systematically characterized with respect to performance and short-term stability as electrolyte in a zero-gap alkaline water electrolyzer at different KOH concentrations. Using plain uncatalyzed nickel foam electrodes, the cell based on m-PBI outperforms the cell based on the commercially available state-of-the-art diaphragm and reaches a current density of 1500 mA cm^{-2} at 2.4 V in 20 wt% KOH at 80°C. The cell performance remained stable during two days of operation, though post analysis of the membrane using size exclusion chromatography and spectroscopy reveal evidence of oxidative degradation of the base polymer at KOH concentrations of 15 wt% and higher.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors
Authors: Kraglund, M. R. (Intern), Aili, D. (Intern), Jankova Atanasova, K. (Intern), Christensen, E. (Intern), Li, Q. (Intern), Jensen, J. O. (Intern)
Number of pages: 7
Pages: F3125-F3131
Publication date: 2016
Main Research Area: Technical/natural sciences
Method for producing and controlling the morphology of metal-oxide nanofiber and/or nanotube catalysts.

Disclosed herein is a process for the controlled production of metal-containing nanofibers and/or nanotubes, where the morphology of the nanofibers and/or nanotubes is followed in real time by TEM measurements.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Risø National Laboratory for Sustainable Energy, Department of Chemistry, Proton conductors
Authors: Zhang, W. (Intern), Esposito, V. (Intern), Ramousse, S. (Intern), Jensen, J. O. (Intern)
Publication date: 12 Nov 2015

Publication information
IPC: D01F 9/08 A1
Patent number: WO2015169786
Date: 12/11/2015
Priority date: 06/05/2014
Priority number: EP20140167202
Original language: English
Electronic versions:
WO2015169786A1.pdf
Main Research Area: Technical/natural sciences
Source: espacenet
Source-ID: WO2015169786
Publication: Research › Patent – Annual report year: 2016

An active magnetic regenerator device
A rotating active magnetic regenerator (AMR) device comprising two or more regenerator beds, a magnet arrangement and a valve arrangement. The valve arrangement comprises a plurality of valve elements arranged substantially immovably with respect to the regenerator beds along a rotational direction. A cam surface is arranged substantially immovably with respect to the magnet arrangement along the rotational direction, and comprises a plurality of cam elements arranged to cooperate with the valve elements in order to control opening degrees of the valve elements, in accordance with a relative position of the cam elements and the valve elements. Thereby the opening degree of each valve element is controlled in accordance with a relative angular position of the regenerator beds and the magnet arrangement.

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy, Department of Energy Conversion and Storage, Electrofunctional materials, Department of Physics
Authors: Eriksen, D. (Intern), Engelbrecht, K. (Intern), Bahl, C. (Intern)
Publication date: 13 Aug 2015
Oxygen transport membrane.
The present invention relates to a novel composite oxygen transport membrane as well as its preparation and uses thereof.

General information
State: Published
Organisations: Mixed Conductors, Department of Energy Conversion and Storage, Ceramic Engineering & Science, Risø National Laboratory for Sustainable Energy
Publication date: 30 Jul 2015

Method for Producing Substrates for Superconducting Layers
There is provided a method for producing a substrate suitable for supporting an elongated superconducting element, wherein one or more elongated strips of masking material are placed on a solid element (202) so as to form one or more exposed elongated areas being delimited on one or two sides by elongated strip of masking material, and placing filling material on the solid element so that each exposed elongated area within the one or more exposed elongated areas is covered by a portion of filling material (318a-c) where each portion of filling material also covers at least a portion of the adjacent elongated strip of masking material and subsequently removing the one or more elongated strips of masking material so as to form one or more corresponding undercut volumes, where each undercut volume within the one or more undercut volumes is formed along a portion of filling material and between the portion of filling material and the solid element. The method may further comprise placing buffer material (640) and or superconducting material (642, 644, 646)) on the substrate, so as to provide a superconducting structure (601) with reduced AC losses.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Authors: Wulff, A. C. (Intern)
Publication date: 28 May 2015
System for cooling a cabinet
The present disclosure relates to a cooling system comprising an active magnetic regenerator having a cold side and a hot side, a hot side heat exchanger connected to the hot side of the magnetic regenerator, one or more cold side heat exchangers, and a cold store reservoir comprising a volume of heat transfer fluid and connected between said one or more cold side heat exchangers and the cold side of the magnetic regenerator, wherein the cooling system is configured to provide a first flow cycle of said heat transfer fluid between the cold store reservoir, the magnetic regenerator and the hot side heat exchanger adapted to transfer thermal energy from the cold store reservoir to the hot side heat exchanger; and at least a second flow cycle of said heat transfer fluid between the cold store reservoir and said one or more cold side heat exchangers adapted to transfer thermal energy from said one or more cold side heat exchangers to the cold store reservoir.

General information
State: Published
Organisations: Risø National Laboratory for Sustainable Energy, Department of Energy Conversion and Storage, Secretariat, IT, Department of Physics, Electrofunctional materials
Authors: Smith, A. (Intern), Bahl, C. (Intern), Linderoth, S. (Intern)
Publication date: 21 May 2015

Publication information
Patent number: WO2015071460
Priority date: 18/11/2013
Priority number: EP20130193332
Original language: English
Electronic versions:
WO2015071460A2.pdf

Searching for electrolytes and electrodes for CO₂ reduction below 300 °C
Electrochemical CO₂ reduction research is driven by the desire to reduce reliance on fossil fuels and lower greenhouse gas emissions. The conversion of CO₂ into fuels and chemicals using energy derived from a renewable source, such as wind or solar, could replace the use of fossil fuels.

This thesis uses the knowledge derived from earlier investigations on electrolysis techniques as the foundation for an exploratory work to find acceptable materials and fabricate an electrochemical cell able to produce hydrocarbons and alcohols directly from reduction of CO₂ and steam. The operating conditions should be between 200 – 300 °C and at elevated pressure in the range of 20 – 30 bar. The temperature range is chosen according to the thermal stability of the hydrocarbons produced by conversion of CO₂. The electrochemical performance of the fabricated cells was evaluated using electrochemical impedance spectroscopy and chronoamperometry, while the gas analysis was carried out via gas chromatography.

The initial part of the study focused on electrolyte materials in order to identify a promising candidate to be implemented in the full cells. Some proton conducting materials, such as Y-doped BaZrO₃-BaCeO₃ solid solutions and K-doped BaZr₁₋ₓYₓO₃₋δ were evaluated. BaCe₀.₅Zr₀.₄Y₀.₁O₃₋δ would have been the best electrolyte candidate because of its low resistivity in high pH₂O (2 · 10⁻³ S/cm) even at temperatures as low as 240 °C. However, the instability in the acidic CO₂ gas atmosphere hinders practical application for carbon dioxide reduction at high pressure. K-doped BaZr₁₋ₓYₓO₃₋δ was successfully synthesized by hydrothermal technique, but the conductivity recorded in high pH₂O and at 240 °C was too low (3 · 10⁻⁵ S/cm) to be considered as a suitable electrolyte.

A literature survey showed that most CO₂ reduction studies were performed in aqueous potassium bicarbonate (KHCO₃) and with a copper metal catalyst. Therefore, it was decided to investigate the electrocatalytic activity of copper foam in
aqueous media at ambient conditions for electrochemical reduction of CO2. The measurements were conducted at Stanford University – Chemical Engineer Department, where it was possible to utilize an experimental setup which ensures high sensitivity for minor products from the CO2 reduction reaction. Seven products were identified with the copper foam electrode tested to -0.98 V vs. RHE. H2, formate and CO were the main products observed and in particular the faradaic efficiency of H2 was ca. 90 %. The highest current density that could be sustained with this setup was about -20 mA/cm2. Therefore, it was decided to develop a new cell that could operate at higher current densities, pressures and temperatures.

A foam based CO2 conversion cell with gas diffusion electrodes and a ceramic porous structure in which the liquid electrolyte is immobilized by capillary forces was developed and tested up to 20 bar and to a maximum temperature of 50 °C. Potassium carbonate was selected as aqueous electrolyte and various concentrations of this electrolyte were immobilized in a ceramic porous matrix at both ambient and elevated temperatures and pressures. Copper and silver metal foams were tested as cathode. Nickel metal foam was chosen as anode. When copper was used as electrocatalyst, a high faradaic efficiency for the evolution of H2, i.e. between 92 to 99 % was registered. The other products detected were CO and during one test also methane was identified. The performance of Ag cathode metal foam confirmed its higher selectivity for CO2 reduction to CO. The formation of passive oxide layers and the subsequent degradation of nickel foam electrodes affected the electrochemical performance and the stability of the cells negatively.

**General information**
State: Published
Organisations: Department of Energy Conversion and Storage, Fundamental Electrochemistry
Authors: Vico, F. (Intern), Mogensen, M. B. (Intern), Chatzichristodoulou, C. (Intern), Holtappels, P. (Intern)
Number of pages: 148
Publication date: May 2015

**Publication information**
Publisher: Department of Energy Conversion and Storage, Technical University of Denmark
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
Searching_for_electrolytes.pdf

**Relations**
Projects:
Searching for electrolytes and electrodes for CO2 reduction below 300 °C
Publication: Research › Ph.D. thesis – Annual report year: 2015

**Elektrolyse gør al energi fra vindmøller værdifuld**

**General information**
State: Published
Organisations: Department of Energy Conversion and Storage, Fundamental Electrochemistry, Applied Electrochemistry, Imaging and Structural Analysis
Publication date: 20 Jan 2015

**Publication information**
Source/Publisher: Videnskab.dk
Main Research Area: Technical/natural sciences
Electronic versions:
Elektrolyse_g_r_al_energi.pdf
Links:
Source: PublicationPreSubmission
Source-ID: 104791703
Publication: Communication › Internet publication – Annual report year: 2015

**1,2,4-Triazolium perfluorobutanesulfonate as an archetypal pure protic organic ionic plastic crystal electrolyte for all-solid-state fuel cells**

1,2,4-Triazolium perfluorobutanesulfonate (1), a novel, pure protic organic ionic plastic crystal (POIPC) with a wide plastic crystalline phase, has been explored as a proof-of-principle anhydrous proton conductor for all-solid-state high temperature hydrogen/air fuel cells. Its physicochemical properties, including thermal, mechanical, structural, morphological, crystallographic, spectral, and ion-conducting properties, as well as fuel cell performances, have been studied comprehensively in both fundamental and device-oriented aspects. With superior thermal stability, 1 exhibits crystal (phase III), plastic crystalline (phase II and I) and melt phases successively from 173 C to 200 C. Differential
scanning calorimetry and temperature dependent powder X-ray diffraction (XRD) measurements together with polarized optical microscopy and thermomechanical analysis reveal the two solid–solid phase transitions of 1 at 76.8°C and 87.2°C prior to the melting transition at 180.9°C, showing a wide plastic phase (87–181°C). Scanning electron microscopy displays the morphology of different phases, indicating the plasticity in phase I. Single-crystal XRD studies reveal the molecular structure of 1 and its three-dimensional N–H/O hydrogen bonding network. The influence of the three-dimensional hydrogen bonding network on the physicochemical properties of 1 has been highlighted. The temperature dependence of hydrogen bonding is investigated by variable-temperature infrared spectroscopy. The sudden weakening of hydrogen bonds at 82°C seems to be coupled with the onset of orientational or rotational disorder of the ions. The temperature dependence of ionic conductivity in the solid and molten states is measured via impedance spectroscopy and current interruption technique, respectively. The Arrhenius plot of the ionic conductivity assumes a lower plateau region (phase I, 100–155°C) with a low activation energy of 36.7 kJ mol⁻¹ (i.e. 0.38 eV), suggesting likely a Grothuss mechanism for the proton conduction. Variable-temperature infrared analysis, optical morphological observations, and powder XRD patterns further illustrate the structural changes. Electrochemical hydrogen pumping tests confirm the protonic nature of the ionic conduction observed in the lower plateau region. Finally, measurements of the open circuit voltages (OCVs) and the polarization curves of a dry hydrogen/air fuel cell prove the long-range proton conduction. At 150°C, a high OCV of 1.05 V is achieved, approaching the theoretical maximum (1.11 V).
Accelerated Degradation for Hardware in the Loop Simulation of Fuel Cell-Gas Turbine Hybrid System

The U.S. Department of Energy (DOE)-National Energy Technology Laboratory (NETL) in Morgantown, WV has developed the hybrid performance (HyPer) project in which a solid oxide fuel cell (SOFC) one-dimensional (1D), real-time operating model is coupled to a gas turbine hardware system by utilizing hardware-in-the-loop simulation. To assess the long-term stability of the SOFC part of the system, electrochemical degradation due to operating conditions such as current density and fuel utilization have been incorporated into the SOFC model and successfully recreated in real time. The mathematical expression for degradation rate was obtained through the analysis of empirical voltage versus time plots for different current densities and fuel utilizations.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry, U.S. DOE National Energy Technology Laboratory, McMaster University
Authors: Abreu-Sepulveda, M. A. (Ekstern), Harun, N. F. (Ekstern), Hackett, G. (Ekstern), Hagen, A. (Intern), Tucker, D. (Ekstern)
Number of pages: 7
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Fuel Cell Science and Technology
Volume: 12
Issue number: 2
Article number: 021001
ISSN (Print): 1550-624X
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Scopus rating (2017): SJR 0.273 SNIP 0.517
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.231 SNIP 0.498 CiteScore 0.74
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.246 SNIP 0.456 CiteScore 0.52
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.308 SNIP 0.458 CiteScore 0.66
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.319 SNIP 0.481 CiteScore 0.64
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.348 SNIP 0.413 CiteScore 0.68
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.395 SNIP 0.451 CiteScore 0.75
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.447 SNIP 0.628
Accelerated DFT-Based Design of Materials for Ammonia Storage

Future energy carriers are needed in order to lower the CO2 emissions resulting from the burning of fossil fuels. One possible energy carrier is ammonia, which can be stored safely and reversibly in metal halide ammines; however, the release often occurs in multiple steps at too high temperatures. Therefore, there is a need for new materials, releasing the ammonia in a narrow temperature interval. To search for new mixed metal halide chlorides, we use DFT calculations guided by a genetic algorithm (GA) to expedite the search, as the defined search space allowing up to three different metals contains more than 100,000 different structures. Here, we search for materials releasing the ammonia between 0 and 100 °C, a temperature range suitable for system integration with low-temperature polymer electrolyte membrane fuel cells (PEMFC). The efficiency of the implemented algorithm is verified by three trial runs capable of finding the same optimal mixtures starting from different random populations, testing <5% of the candidates. Some of the best candidates are already confirmed experimentally, and others offer a record high, accessible hydrogen capacity exceeding 9 wt %.

Among the identified materials is the first known high-capacity ternary metal halide ammine, which we have subsequently synthesized and confirmed the ammonia storage properties using temperature-programmed desorption (TPD).
Accelerated testing of solid oxide fuel cell stacks for micro combined heat and power application

State-of-the-art (SoA) solid oxide fuel cell (SOFC) stacks are tested using profiles relevant for use in micro combined heat and power (CHP) units. Such applications are characterised by dynamic load profiles. In order to shorten the needed testing time and to investigate potential acceleration of degradation, the profiles are executed faster than required for real applications. Operation with fast load cycling, both using hydrogen and methane/steam as fuels, does not accelerate degradation compared to constant operation, which demonstrates the maturity of SoA stacks and enables transferring knowledge from testing at constant conditions to dynamic operation. 7.5 times more cycles than required for \( 80,000 \) h lifetime as micro CHP are achieved on one-cell-stack level. The results also suggest that degradation mechanisms that proceed on a longer time-scale, such as creep, might have a more dominating effect for long life-times than regular short time changes of operation. In order to address lifetime testing it is suggested to build a testing program consisting of defined modules that represent different application profiles, such as one module at constant conditions, followed by modules at one set of dynamic conditions etc.
Acid-base Chemistry and Proton Conductivity of High Temperature Polymer Electrolytes

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors
Authors: Li, Q. (Intern), Aili, D. (Intern), Cleemann, L. N. (Intern), Jensen, J. O. (Intern)
Number of pages: 1
Publication date: 2015
Main Research Area: Technical/natural sciences

Bibliographical note
Oral by Qingfeng Li
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2016

Acido-basic control of the thermoelectric properties of poly(3,4-ethylenedioxythiophene)tosylate (PEDOT-Tos) thin films
PEDOT-Tos is one of the conducting polymers that displays the most promising thermoelectric properties. Until now, it has been utterly difficult to control all the synthesis parameters and the morphology governing the thermoelectric properties. To improve our understanding of this material, we study the variation in the thermoelectric properties by a simple acid-base treatment. The emphasis of this study is to elucidate the chemical changes induced by acid (HCl) or base (NaOH) treatment in PEDOT-Tos thin films using various spectroscopic and structural techniques. We could identify changes in the nanoscale morphology due to anion exchange between tosylate and Cl- or OH-. But, we identified that changing the pH leads to a tuning of the oxidation level of the polymer, which can explain the changes in thermoelectric properties. Hence, a simple acid-base treatment allows finding the optimum for the power factor in PEDOT-Tos thin films.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Imaging and Structural Analysis, Linköping University, University of South Australia
Number of pages: 8
Pages: 10616-10623
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Materials Chemistry C
Volume: 3
Activated Carbon Nanochains with Tailored Micro-Meso Pore Structures and Their Application for Supercapacitors

Carbon nanochains (CNCs) were synthesized by a facile chemical vapor deposition process consisting of a 1D chain of interconnected carbon nano-onions for potential application in supercapacitors. In this study, the CNCs were further activated by a chemical method using potassium hydroxide (KOH) as the activation agent to obtain micro-meso pore structures. To improve the specific surface area (SSA) and optimize the pore size distribution (PSD) to enhance the capacitance performance, we investigated the activation parameters, including the KOH content, temperature and duration. The results indicated that CNCs with a hierarchical pore structure and high SSA could be achieved using an activation process with a KOH-to-CNC ratio of 2 at 900 degrees C for 20 h. The mechanism is also discussed. The activation temperature and duration affect the promotion of the carbon graphitization and exaggeration of the carbon etching. The CNCs activated using the optimal parameters exhibited a high capacitance performance of 112.7 F g(-1) at 50 mV s(-1) with excellent stability in 6 M KOH electrolyte, which was due to the improved surface and micromesoporosity without sacrificing their electronic transmission properties.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors, Tianjin University
Authors: Zhang, M. (Ekstern), He, C. (Ekstern), Liu, E. (Ekstern), Zhu, S. (Ekstern), Shi, C. (Ekstern), Li, J. (Ekstern), Li, Q. (Intern), Zhao, N. (Ekstern)
Number of pages: 8
Pages: 21810-21817
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Physical Chemistry C
Volume: 119
Issue number: 38
ISSN (Print): 1932-7447
Ratings:
BFI (2018): BFI-level 1
High Temperature (HT) wellbores represent one of today’s biggest challenges for the oil and gas industry. The majority of well intervention wireline tools contain temperature sensitive electronics that are not able to withstand the high temperatures of HT wellbores (> 150 °C), for an extended period of time. This work presents the design and construction of an actively cooled laboratory prototype, which is able to operate at temperatures which are higher than the temperature limit of the electronics. A different concept of heat management, compared to prior works, is presented: the design combines active and passive cooling techniques, aiming at an efficient thermal management, preserving the tool
compactness and avoiding the use of moving parts. Thermoelectric coolers were used to transfer the dissipated heat from the temperature-sensitive electronics to the external environment. Thermal contact resistances were minimized and thermally insulating foam protected the refrigerated microenvironment from the hot surroundings.

**A DFT-based genetic algorithm search for AuCu nanoalloy electrocatalysts for CO2 reduction**

Using a DFT-based genetic algorithm (GA) approach, we have determined the most stable structure and stoichiometry of a 309-atom icosahedral AuCu nanoalloy, for potential use as an electrocatalyst for CO2 reduction. The identified core–shell nano-particle consists of a copper core interspersed with gold atoms having only copper neighbors and a gold surface with a few copper atoms in the terraces. We also present an adsorbate-dependent correction scheme, which enables an accurate determination of adsorption energies using a computationally fast, localized LCAO-basis set. These show that it is possible to use the LCAO mode to obtain a realistic estimate of the molecular chemisorption energy for systems where the computation in normal grid mode is not computationally feasible. These corrections are employed when calculating adsorption energies on the Cu, Au and most stable mixed particles. This shows that the mixed Cu135@Au174 core–shell nanoalloy has a similar adsorption energy, for the most favorable site, as a pure gold nano-particle. Cu, however, has the effect of stabilizing the icosahedral structure because Au particles are easily distorted when adding adsorbates.
Photovoltaic devices based on organic semiconductors (OPVs) hold great promise as a cost-effective renewable energy platform because they can be processed from solution and deposited on flexible plastics using roll-to-roll processing. Despite important progress and reported power conversion efficiencies of more than 10% the rather limited stability of this type of devices raises concerns towards future commercialization. The tandem concept allows for both absorbing a broader range of the solar spectrum and reducing thermalization losses. We designed an organic tandem solar cell with an inverted device geometry comprising environmentally stable active and charge-selecting layers. Under continuous white light irradiation, we demonstrate an extrapolated, operating lifetime in excess of one decade. We elucidate that for the current generation of organic tandem cells one critical requirement for long operating lifetimes consists of periodic UV
light treatment. These results suggest that new material approaches towards UV-resilient active and interfacial layers may enable efficient organic tandem solar cells with lifetimes competitive with traditional inorganic photovoltaics.

General information
State: Published
Authors: Adams, J. (Ekstern), Spyropoulos, G. D. (Ekstern), Salvador, M. (Ekstern), Li, N. (Ekstern), Strohm, S. (Ekstern), Lucera, L. (Ekstern), Langner, S. (Ekstern), Machui, F. (Ekstern), Zhang, H. (Ekstern), Ameri, T. (Ekstern), Voigt, M. M. (Ekstern), Krebs, F. C. (Intern), Brabec, C. J. (Ekstern)
Number of pages: 8
Pages: 169-176
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Energy & Environmental Science
Volume: 8
Issue number: 1
ISSN (Print): 1754-5692
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): SNIP 4.819 SJR 14.59 CiteScore 30.87
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 26.39 SJR 12.283 SNIP 4.325
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 7.769 SNIP 4.001 CiteScore 19.28
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 6.019 SNIP 2.996 CiteScore 14.81
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 5.868 SNIP 2.599 CiteScore 11.84
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 3.737 SNIP 2.505 CiteScore 9.96
ISI indexed (2011): ISI indexed no
Web of Science (2011): Indexed yes
Scopus rating (2010): SJR 3.87 SNIP 2.42
Web of Science (2010): Indexed yes
Scopus rating (2009): SJR 2.111 SNIP 1.15
Original language: English
DOIs:
10.1039/c4ee02582b
Source: FindIt
Source-ID: 270992894
Publication: Research - peer-review › Journal article – Annual report year: 2015
Alkali Metal-O₂ Batteries. Performance and Lifetime Limiting Effects
The rechargeable Na-O₂ and Li-O₂ batteries are attractive battery technologies as they potentially are very cheap and as they theoretically possess about 3 and 10 times higher energy density than the current Li-ion technologies. This PhD thesis is dedicated to studying the effects that limit cell performance of these two technologies.

The Li-O₂ battery was first introduced in 1996 and focus in the field is still on understanding the fundamental mechanisms controlling discharge and charge. This PhD thesis was mainly dedicated to the Li-O₂ battery and initially charge conduction through the discharge product, Li₂O₂, was investigated. This was done by using of a conventional three electrode cell in which the heterogeneous electron transfer rate of three different redox couples were studied on Li₂O₂ coated glassy carbon electrodes to provide a measure of the conductivity of the Li₂O₂ layers. Charge transport through Li₂O₂ gives further evidence that hole transport dominates charge-transfer through Li₂O₂. Electrochemical impedance spectroscopy was also used to conduct detailed investigations of surface capacitance, ion transport, and charge-transfer reactions in the cathode of the Li-O₂ cell. The capacitance of the cathode was shown to be sensitive to the thickness of the deposited Li₂O₂ layer. These investigations also explored the influence of the composition of the electrolyte and conditions, which favors a solution mediated Li₂O₂ deposition mechanism. On charge, an electrochemical “safe” operating voltage was identified until 3.30 V were an interface layer was formed, which activates side reactions and further increases the cell potential. A number of ionic liquids were also investigated for their oxygen diffusivity and solubility and while these were in the order of currently employed aprotic electrolytes as the ionic liquids significantly decompose under electrochemical operation. Last, the influence of CO₂ was investigated and it was suggested that CO₂ blocks the step valleys of the deposited Li₂O₂ forcing Li₂O₂ growth away from the electrode surface hereby increasing cell capacity, as the discharge becomes less limited by the cathode surface area.

The Na-O₂ battery is an even newer technology as it was first introduced to the scientific community in 2010. The two batteries are experimentally quite similar as the only difference is the choice of anode. However, when one studies the two systems, the mechanisms controlling each type of battery are quite different. The discharge and charge processes of the non-aqueous Na-O₂ battery were studied in this thesis. On discharge, the deposition mechanism of NaO₂ was shown to be highly dependent on the current density and cell limitations could be correlated to the depositions mechanisms. On charge, three regions of NaO₂ oxidation were identified, each corresponding to a different type of NaO₂ oxidation.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, Applied Electrochemistry
Authors: Knudsen, K. B. (Intern), Hjelm, J. (Intern), Jensen, S. H. (Intern), Holtappels, P. (Intern)
Number of pages: 193
Publication date: 2015

Publication information
Place of publication: Kgs. Lyngby
Publisher: Department of Energy Conversion and Storage, Technical University of Denmark
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
Kristian_B_Knudsen_Alkali_Metal_oxygen_Batteries_PhD_Thesis.pdf

Relations
Projects:
Alkali Metal-O₂ Batteries. Performance and Lifetime Limiting Effects
Source: PublicationPreSubmission
Source-ID: 134708070
Publication: Research › Ph.D. thesis – Annual report year: 2015

Alkalisk elektrolyse til vedvarende energikilder

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Imaging and Structural Analysis
Authors: Bowen, J. R. (Intern)
Number of pages: 1
Pages: 27-27
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: FIB - Forskning i Bioenergi, Brint & Brændelsceller
Volume: 12
Ambient effects on the electrical conductivity of carbon nanotubes

We show that the electrical conductivity of single walled carbon nanotubes (SWCNT) networks is affected by oxygen and air humidity under ambient conditions by more than a magnitude. Later, we intentionally modified the electrical conductivity by functionalization with iodine and investigated the changes in the band structure by optical absorption spectroscopy. Measuring in parallel the tubes electrical conductivity and optical absorption spectra, we found that conduction mechanism in SWCNT is comparable to that of intrinsically conducting polymers. We identified, in analogy to conducting polymers, in the infrared spectra a new absorption band which is responsible for the increased conductivity, leading to a closing gap in semiconducting SWCNT. We could show that by different functionalizations of the same SWCNT starting material the properties like conductivity can be dramatically changed, leading to different imaginable applications. We investigated here, an ultraviolet sensor with weakly modified SWCNT.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Dresden University of Technology, Fraunhofer Institute for Material and Beam Technology
Authors: Roch, A. (Ekstern), Greifzu, M. (Ekstern), Roch Talens, E. (Ekstern), Stepien, L. (Ekstern), Roch, T. (Ekstern), Hege, J. (Ekstern), Van Nong, N. (Intern), Schmiel, T. (Ekstern), Dani, I. (Ekstern), Leyens, C. (Ekstern), Jost, O. (Ekstern), Leson, A. (Ekstern)
Pages: 347-353
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Carbon
Volume: 95
ISSN (Print): 0008-6223
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SJR 2.226 SNIP 1.666 CiteScore 6.76
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 6.49 SJR 2.091 SNIP 1.648
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.988 SNIP 1.71 CiteScore 6.53
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.132 SNIP 1.976 CiteScore 6.62
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 2.289 SNIP 2.114 CiteScore 6.54
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.518 SNIP 2.102 CiteScore 5.95
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.193 SNIP 2.048 CiteScore 5.23
ISI indexed (2011): ISI indexed yes
A model for the impact of the nanostructure size on its gas sensing properties

The size of a metal oxide nanostructure plays a key role in its performance as a gas sensor. ZnO nanostructures with different morphologies including nanowires at different diameters and nanodisks at different thicknesses were synthesized hydrothermally. Gas sensors based on individual nanostructures with different sizes were fabricated and their sensing properties were compared and investigated. Nanowires with smaller diameter size and higher surface to volume ratio showed enhanced gas sensing performance. Also, as the nanodisk thickness gets closer to the thickness of the ZnO depletion layer, the sensitivity increases significantly due to the semi complete depletion of the nanostructure. Our results were explained using a modified general formula for a ZnO ethanol sensor. The formula was established based on the chemical reaction between ethanol molecules and oxygen ions and considering the effect of the surface to volume ratio as well as the depletion region of the nanostructure. This work can be simply generalized for other metal oxides to enhance their performance as gas sensors.
Analysis of the Interphase on Carbon Black Formed in High Voltage Batteries

Carbon black (CB) additives commonly used to increase the electrical conductivity of electrodes in Li-ion batteries are generally believed to be electrochemically inert additives in cathodes. Decomposition of electrolyte in the surface region of CB in Li-ion cells at high voltages up to 4.9 V is here studied using electrochemical measurements as well as structural and surface characterizations. LiPF$_6$ and LiClO$_4$ dissolved in ethylene carbonate:diethylene carbonate (1:1) were used as the electrolyte to study irreversible charge capacity of CB cathodes when cycled between 4.9 V and 2.5 V. Synchrotron-based soft X-ray photoelectron spectroscopy (SOXPES) results revealed spontaneous partial decomposition of the electrolytes on the CB electrode, without applying external current or voltage. Depth profile analysis of the electrolyte/cathode interphase indicated that the concentration of decomposed species is highest at the outermost surface of the CB. It is concluded that carboxylate and carbonate bonds (originating from solvent decomposition) and LiF (when LiPF$_6$ was used) take part in the formation of the decomposed species. Electrochemical impedance spectroscopy measurements and transmission electron microscopy results, however, did not show formation of a dense surface layer on CB particles.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, Applied Electrochemistry, Imaging and Structural Analysis, Uppsala University
Authors: Younesi, R. (Intern), Christiansen, A. S. (Intern), Scipioni, R. (Intern), Ngo, D. (Intern), Simonsen, S. B. (Intern), Edström, K. (Ekstern), Hjelm, J. (Intern), Norby, P. (Intern)
Pages: A1289-A1296
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of The Electrochemical Society
Volume: 162
Issue number: 7
ISSN (Print): 0013-4651
Ratings:
Analysis of the Interphase on Carbon Black Formed in High Voltage Batteries

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, Applied Electrochemistry, Imaging and Structural Analysis, Uppsala University
Authors: Younesi, R. (Intern), Christiansen, A. S. (Intern), Scipioni, R. (Intern), Ngo, D. (Intern), Simonsen, S. B. (Intern), Edström, K. (Ekstern), Hjelm, J. (Intern), Norby, P. (Intern)
Number of pages: 1
Publication date: 2015
Main Research Area: Technical/natural sciences

An efficient numerical scheme for the simulation of parallel-plate active magnetic regenerators
A one-dimensional model of a parallel-plate active magnetic regenerator (AMR) is presented in this work. The model is based on an efficient numerical scheme which has been developed after analysing the heat transfer mechanisms in the regenerator bed. The new finite difference scheme optimally combines explicit and implicit techniques in order to solve the one-dimensional conjugate heat transfer problem in an accurate and fast manner while ensuring energy conservation. The present model has been thoroughly validated against passive regenerator cases with an analytical solution. Compared to the fully implicit scheme, the proposed scheme achieves more accurate results, prevents numerical errors and requires less computational effort. In AMR simulations the new scheme can reduce the computational time by 88%.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Universidad Politecnica de Valencia
Authors: Torregrosa-Jaime, B. (Ekstern), Corberán, J. M. (Ekstern), Payá, J. (Ekstern), Engelbrecht, K. (Intern)
Pages: 121-130
Publication date: 2015
Main Research Area: Technical/natural sciences
An Electrochemical Impedance Spectroscopy Investigation of the Overpotentials in Li−O2 Batteries

Lithium−O2 (Li−O2) batteries are currently limited by a large charge overpotential at practically relevant current densities, and the origin of this overpotential has been heavily debated in the literature. This paper presents a series of electrochemical impedance measurements suggesting that the increase in charge potential is not caused by an increase in the internal resistance. It is proposed that the potential shift is instead dictated by a mixed potential of parasitic reactions and Li2O2 oxidation. The measurements also confirm that the rapid potential loss near the end of discharge (“sudden death”) is explained by an increase in the charge transport resistance. The findings confirm that our theory and conclusions in ref 1, based on experiments on smooth small-area glassy carbon cathodes, are equally valid in real Li−O2 batteries with porous cathodes. The parameter variations performed in this paper are used to develop the understanding of the electrochemical impedance, which will be important for further improvement of the Li−air battery.
An investigation on the role of thermal fins in the design of micro heat exchangers

The different dominant physical phenomena in design for micro and macro scale products result in different design considerations for both categories. In the current study, a few design concepts are proposed as micro heat exchangers. In addition, the influential parameters on design of a micro heat exchanger in comparison with the effective factors in designing its macro counterpart are investigated. Numerical simulations in the finite element software COMSOL are used to evaluate the thermal performance of both micro and macro heat exchangers. The result of the analysis reveals the fact that the presence of some features such as “fins” in micro heat exchanger is not as significant as it is in macro scale. The results of this study can be employed as guidelines in design of similar micro heat exchangers.
An isoindigo containing donor-acceptor polymer: synthesis and photovoltaic properties of all-solution-processed ITO- and vacuum-free large area roll-coated single junction and tandem solar cells

In this work, the design, synthesis, and characterization of a donor-acceptor polymer from dithieno[3,2-b:2',3'-d]pyrrole and isoindigo (i-ID) are presented. The synthesized polymer has been applied in large area ITO-free organic photovoltaics, both as spin coated and roll coated devices; the latter as both single junction and multi junction organic photovoltaic (OPV) architectures.
Anode Support Creep
Initial reduction temperature of an SOC is kept higher than the highest intended operation temperature of the SOC to keep
the electrolyte under compression by the Anode Support at all temperatures equal to and below the maximum intended
operation temperature.

A novel CO₂- and SO₂-tolerant dual phase composite membrane for oxygen separation
A novel dual phase composite oxygen membrane (Al₀.₀₂Ga₀.₀₂Zn₀.₉₆O₁.₀₂ − Gd₀.₁Ce₀.₉O₁.₉₅₋δ) was successfully
prepared and tested. The membrane shows chemical stability against CO₂ and SO₂, and a stable oxygen permeation
over 300 hours in CO₂ was demonstrated. ZnO is cheap and non-toxic and is therefore highly advantageous compared to
other common materials used for the purpose.
Assessment of (Mn,Co)₃O₄ powders for possible coating material for SOFC/SOEC Interconnects

In this work (Mn,Co)₃O₄ spinel powders with different Mn:Co ratio (1:1 and 1:2) and from different commercial suppliers are evaluated for possible powder for production of interconnect coatings. Sinterability of the powders is evaluated on pressed pellets sintered in oxidizing and in reducing/oxidizing atmospheres. For selected powder, coatings are then prepared by the electrophoretic deposition method on Crofer 22 APU stainless steel coupons. Effects of dispersant/iodine content and deposition voltage and times are evaluated. Thickness as a function of deposition parameters is described. Results show that with appropriate powder it is possible to produce adherent protective coating with a well-controlled thickness.

General information

State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Gdansk University of Technology
Authors: Szymczewska, D. (Ekstern), Molin, S. (Intern), Venkatachalam, V. (Intern), Chen, M. (Intern), Jasinski, P. (Ekstern), Hendriksen, P. V. (Intern)
Number of pages: 9
A Study of $e^-$ Transport through Li$_2$O$_2$, the Main Discharge Product in the Li-O$_2$ Battery

In the field of energy storage devices, the pursuit for cheap, high energy density, reliable secondary batteries is at the top of the agenda. The Li-O$_2$ battery is one of the possible technologies that, in theory, should be able to close the gap, which exists between the present state-of-the-art Li-ion technologies and the demand placed on batteries by technologies such as electrical vehicles [1]. However, the Li-O$_2$ battery still suffers greatly from high overpotentials during oxygen reduction and evolution reactions (discharge and charge, respectively), poor rechargeability, and decomposition of salts and solvents etc. [2] [3]. In order to improve the electrochemical performance of the Li-O$_2$ batteries, it is crucial to understand the fundamental mechanisms that govern and limit the system during electrochemical operation. Here we present a redox probing study of the charge transfer across the deposition product lithium peroxide, Li$_2$O$_2$, using outer-sphere redox shuttles: cobaltocene, ferrocene, and decamethylferrocene. The change in heterogeneous electron transfer exchange rate as a function of the potential and the Li$_2$O$_2$ layer thickness (~state of charge) was determined using electrochemical impedance spectroscopy. The attenuation of the electron transfer exchange rate with film thickness is dependent on the probing potential, indicating that hole tunneling is the dominant process for charge transfer through Li$_2$O$_2$ supporting previous work by Luntz et al. [4]. Additionally, this work includes the determination of diffusion coefficients and concentrations of the redox shuttles and the superoxide ion, in a 1,2-dimethoxyethane based electrolyte. The change in heterogeneous electron transfer exchange rate as a function of the potential and the Li$_2$O$_2$ layer thickness (~state of charge) was determined using electrochemical impedance spectroscopy. The attenuation of the electron transfer exchange rate with film thickness is dependent on the probing potential, indicating that hole tunneling is the dominant process for charge transfer through Li$_2$O$_2$ supporting previous work by Luntz et al. [4].

References
A study of thermoelectric $\beta$-Zn$_4$Sb$_3$ under thermal cycling and large temperature gradients

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, TEGnology ApS, Aarhus University
Authors: Le, T. H. (Intern), Van Nong, N. (Intern), Han, L. (Intern), Brummerstedt Iversen, B. (Ekstern), Yin, H. (Forskerdatabase), Pryds, N. (Intern)
Publication date: 2015
Host publication information
Title of host publication: Book of Abstracts - 34th Annual International Conference on Thermoelectrics (ICT 2015) and 13th European conference on Thermoelectrics (ECT 2015)
Article number: PA188
Main Research Area: Technical/natural sciences
Conference: 34th Annual International Conference on Thermoelectrics (ICT 2015) and 13th European conference on Thermoelectrics (ECT 2015), Dresden, Germany, 28/06/2015 - 28/06/2015
Electronic versions:
ITC2015_Book_of_Abstract_07.pdf
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2015

Band bending and alignment at the spinel/perovskite $\gamma$-Al$_2$O$_3$/SrTiO$_3$ heterointerface

We present a comprehensive study of the band bending and alignment at the interface of $\gamma$-Al$_2$O$_3$/SrTiO$_3$ heterostructures by hard x-ray photoelectron spectroscopy. Our measurements find no signs for a potential gradient within the polar $\gamma$-Al$_2$O$_3$ film as predicted by the basic electronic reconstruction scenario. We present evidence for a band bending on the SrTiO$_3$ side of the interface, yielding a roughly 600 meV deep potential trough, which reaches below the chemical potential and has a spatial expansion of 3–5 unit cells. The band offset between the bulk valence bands is determined to be also approximately 600 meV, corresponding to aligned bands at the interface. Finally, the spatial confinement of the interfacial two-dimensional electron system is derived from the chemically shifted Ti3+ photoemission signal in the Ti 2p core level spectra, measured at various photoelectron detection angles. It is found to be in excellent agreement with the spatial depth of the potential trough.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Universität Würzburg, Helmholtz–Zentrum Berlin für Materialien und Energie
Authors: Schütz, P. (Ekstern), Pfaff, F. (Ekstern), Scheiderer, P. (Ekstern), Chen, Y. (Intern), Pryds, N. (Intern), Gorgoi, M. (Ekstern), Sing, M. (Ekstern), Claessen, R. (Ekstern)
Number of pages: 9
Publication date: 2015
Main Research Area: Technical/natural sciences
Publication information
Journal: Physical Review B Condensed Matter
Volume: 91
Issue number: 16
Article number: 165118
ISSN (Print): 0163-1829
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 3.34 SJR 1.604 SNIP 1.04
Web of Science (2017): Indexed yes
Scopus rating (2016): CiteScore 3.16 SJR 2.339 SNIP 1.151
Web of Science (2016): Indexed yes
Scopus rating (2015): SJR 2.377 SNIP 1.13 CiteScore 2.8
Web of Science (2015): Indexed yes
Scopus rating (2014): SJR 2.762 SNIP 1.316 CiteScore 3.3
Web of Science (2014): Indexed yes
Scopus rating (2013): SJR 2.813 SNIP 1.326 CiteScore 3.55
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Scopus rating (2012): SJR 3.173 SNIP 1.378 CiteScore 3.57
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
Scopus rating (2011): SJR 3.326 SNIP 1.423 CiteScore 3.61
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
Scopus rating (2010): SJR 3.318 SNIP 1.447
Web of Science (2010): Indexed yes
Web of Science (2009): Indexed yes
Scopus rating (2008): SJR 2.923 SNIP 1.516
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 2.892 SNIP 1.588
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 2.62 SNIP 1.468
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 2.126 SNIP 1.156
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 2.012 SNIP 1.103
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 2.184 SNIP 1.179
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 2.856 SNIP 1.841
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 3.132 SNIP 1.727
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 2.84 SNIP 1.603
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 2.789 SNIP 1.541
Original language: English
Electronic versions:
Band_bending_and_alignment.pdf
DOIs:
10.1103/PhysRevB.91.165118
Source: PublicationPreSubmission
Source-ID: 107808045
Publication: Research - peer-review › Journal article – Annual report year: 2015
Bipolar polaron pair recombination in P3HT/PCBM solar cells

The unique properties of organic semiconductors make them versatile base materials for many applications ranging from light emitting diodes to transistors. The low spin-orbit coupling typical for carbon-based materials and the resulting long spin lifetimes give rise to a large in uence of the electron spin on charge transport which can be exploited in spintronic devices or to improve solar cell eciencies. Magnetic resonance techniques are particularly helpful to elucidate the microscopic structure of paramagnetic states in semiconductors as well as the transport processes they are involved in. However, in organic devices the nature of the dominant spin-dependent processes is still subject to considerable debate. Using multi-frequency pulsed electrically detected magnetic resonance (pEDMR), we show that the spin-dependent response of P3HT/PCBM solar cells at low temperatures is governed by bipolar polaron pair recombination involving the positive and negative polarons in P3HT and PCBM, respectively, thus excluding a unipolar bipolaron formation as the main contribution to the spin-dependent charge transfer in this temperature regime. Moreover the polaron-polaron coupling strength and the recombination times of polaron pairs with parallel and antiparallel spins are determined. Our results demonstrate that the pEDMR pulse sequences recently developed for inorganic semiconductor devices can very successfully be transferred to the study of spin and charge transport in organic semiconductors, in particular when the dierent polarons can be distinguished spectrally.

Bipolar polaron pair recombination in polymer/fullerene solar cells

We present a study of the rate-limiting spin-dependent charge-transfer processes in different polymer/fullerene bulk-heterojunction solar cells at 10 K. Observing central spin-locking signals in pulsed electrically detected magnetic resonance and an inversion of Rabi oscillations in multifrequency electron-double-resonance spectroscopy, we find that the spin response of both spin-coated and printed P3HT/PCBM and spin-coated PCDTBT/PCBM solar cells at low temperatures is governed by bipolar polaron pair recombination and quantitatively determine the polaron-polaron coupling strength with double electron-electron resonance experiments. Furthermore spin Hahn echo decay and inversion recovery measurements are performed to measure spin coherence and recombination times of the polaron pairs, respectively.
Capillary based Li-air batteries for in situ synchrotron X-ray powder diffraction studies

For Li-air batteries to reach their full potential as energy storage system, a complete understanding of the conditions and reactions in the battery during operation is needed. To follow the reactions in situ a capillary-based Li-O2 battery has been developed for synchrotron-based in situ X-ray powder diffraction (XRPD). In this article, we present the results for the analysis of 1st and 2nd deep discharge and charge for a cathode being cycled between 2 and 4.6 V. The crystalline precipitation of Li2O2 only is observed in the capillary battery. However, there are indications of side reactions. The Li2O2
diffraction peaks grow with the same rate during charge and the development of the full width at half maximum (FWHM) is hkl dependent. The difference in the FWHM of the 100 and the 102 reflections indicate anisotropic morphology of the Li2O2 crystallites or defects along the c-axis. The effect of constant exposure of X-ray radiation to the electrolyte and cathode during charge of the battery was also investigated. X-ray exposure during charge leads to changes in the development of the intensity and the FWHM of the Li2O2 diffraction peaks. The X-ray diffraction results are supported by ex situ X-ray photoelectron spectroscopy (XPS) of discharged cathodes to illuminate non-crystalline deposited materials.
voltage spontaneously increased, thereby indicating cell degradation and possibly the onset of carbon deposition. The outlet gas composition at each current step was estimated based on the inlet gas composition and the reactant conversion using Faraday's law. The increase in voltage was observed at lower pCO/pCO2 ratios than that corresponding to the thermodynamic threshold for carbon formation. Electrochemical impedance spectroscopy in both H2/H2O and CO/CO2 revealed an increase in resistance of the fuel electrode after each CO2 electrolysis current-voltage curve, indicating possible carbon deposition. The difference in partial oxygen pressure between inlet and outlet was analyzed to verify carbon deposition. The increase in voltage is likely due to either blocking of the reaction sites by the deposited carbon, or due to the microstructural damage caused by the carbon, or a combination of these.

Moreover, the current step-size and step-length was varied to investigate the time-dependence of the detection of carbon deposition. Initial results indicate that for longer current steps, carbon formation is observed at lower pCO/pCO2 ratios. This is related to the rate of carbon deposition and the averaged nature of the cell voltage measurements. Possible reasons for these observations will be discussed in detail.

In an attempt to mitigate the degradation due to carbon deposition, the Ni-YSZ electrode was infiltrated with a gadolinium doped ceria (CGO) solution. Initial results indicate that the coking tolerance was not enhanced, but it is still unclear whether infiltrated cells degrade less. However, infiltrated cells display a significant performance enhancement before coking, especially under electrolysis current.

The investigation thus indicated carbon formation in the Ni containing fuel electrode before the thermodynamically calculated threshold for average measurements of the cell was reached. The deviation from the average threshold was reproduced on several cells and quantified (figure 1). The observation of carbon formation on a local, microstructural level before the expected thermodynamic threshold for average measurements on the cell level, is of crucial importance when choosing operating conditions for commercial systems. The effect would be even more severe on stack level, where the gas diffusion and temperature gradients are more pronounced. Initial results of the mitigation strategy of infiltrating CGO are negative, but increased performance prior to coking was observed.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry, Haldor Topsoe AS
Authors: Skafte, T. L. (Intern), Graves, C. R. (Intern), Blennow, P. (Ekstern), Hjelm, J. (Intern)
Number of pages: 9
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Electrochemical Society. Meeting Abstracts (Online)
Volume: MA2015-03
Issue number: 395
ISSN (Print): 2151-2043
Original language: English
Publication: Research - peer-review › Conference abstract in journal – Annual report year: 2015

Carbon Deposition during CO2 Electrolysis in Ni-Based Solid-Oxide-Cell Electrodes
The carbon formation threshold in an operating cell was investigated during electrolysis of an idealized reactant atmosphere of CO and CO2. The electrolysis current was gradually increased in steps until the cell voltage spontaneously increased, thereby indicating cell degradation and possibly the onset of carbon deposition. The outlet gas composition at each current step was estimated based on the inlet gas composition and the reactant conversion using Faraday's law. The increase in voltage was observed at lower outlet pCO/pCO2 ratios than that corresponding to the expected thermodynamic threshold for carbon formation. The degradation observed was related to the fuel electrode, as confirmed by electrochemical impedance spectroscopy. Mitigation of the degradation mechanism was attempted by infiltrating gadolinium doped ceria. The onset of carbon deposition was largely unaffected, but the polarization resistance of the electrode during electrolysis was significantly decreased.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry, Haldor Topsoe AS
Authors: Skaffte, T. L. (Intern), Graves, C. R. (Intern), Blennow, P. (Ekstern), Hjelm, J. (Intern)
Number of pages: 9
Pages: 3429-3437
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Carbon Thin-layer Encapsulated Fe-N-C as Active Catalysts for Oxygen Reduction

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors
Authors: Zhong, L. (Intern), Pan, C. (Intern), Hu, Y. (Intern), Cleemann, L. N. (Intern), Jensen, J. O. (Intern), Li, Q. (Intern)
Number of pages: 1
Publication date: 2015
Main Research Area: Technical/natural sciences

Bibliographical note
Oral by Zhong)
Source: PublicationPreSubmission
Source-ID: 2279821838
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2016

Catalytic Enhancement of Carbon Black and Coal-Fueled Hybrid Direct Carbon Fuel Cells
Hybrid direct carbon fuel cells (HDCFCs) consisting of a solid carbon (carbon black)-molten carbonate ((62–38 wt% Li-K)2CO3) mixtures in the anode chamber of an anode-supported solid oxide fuel cell type full-cell are tested for their
electrochemical performance between 700 and 800°C. Performance was investigated using current-voltage-power density curves. In the anode chamber, catalysts are mixed with the carbon-carbonate mixture. These catalysts include various manganese oxides (MnO2, Mn2O3, Mn3O4, MnO), metal carbonates (Ag2CO3, MnCO3, Ce2(CO3)3), metals (Ag, Ce, Ni), doped-ceria (CeO2, Ce1-xGdxO2-x/2, Ce1-xREExO2-δ (REE = Pr, Sm)) and metal oxides (LiMn2O4, Ag2O). Materials showing the highest activity in carbon black (Mn2O3, CeO2, Ce0.6Pr0.4O2-δ, Ag2O) were subsequently tested for catalytic activity toward bituminous coal, as revealed by both I-V-P curves and electrochemical impedance spectroscopy (EIS). Catalytic activity was evaluated as a function of various physical characteristics of doped ceria and manganese-based materials.

**General information**
State: Published
Organisations: Department of Energy Conversion and Storage, Fundamental Electrochemistry
Authors: Deleebeeck, L. (Intern), Ippolito, D. (Intern), Kammer Hansen, K. (Intern)
Pages: F327-F339
Publication date: 2015
Main Research Area: Technical/natural sciences

**Publication information**
Journal: Journal of the Electrochemical Society
Volume: 162
Issue number: 3
ISSN (Print): 0013-4651
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 3.48 SJR 1.267 SNIP 1.009
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.97 SJR 1.222 SNIP 0.963
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.115 SNIP 1.066 CiteScore 3.17
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.213 SNIP 1.25 CiteScore 3.36
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.169 SNIP 1.309 CiteScore 2.92
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.329 SNIP 1.281 CiteScore 2.61
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.331 SNIP 1.335 CiteScore 2.74
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.418 SNIP 1.304
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.442 SNIP 1.27
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.595 SNIP 1.41
Web of Science (2008): Indexed yes
Catalytic Surface Promotion of Composite Cathodes in Protonic Ceramic Fuel Cells

Composite cathodes based on an electronic conductor and a protonic conductor show advantages for protonic ceramic fuel cells. In this work, the performance of a La$_{5.5}$WO$_{11.25-δ}$/La$_0.8$Sr$_0.2$MnO$_{3+δ}$ (LWO/LSM) composite cathode in a fuel cell based on an LWO protonic conducting electrolyte is shown and catalytically improved. The limiting processes were first unambiguously associated to surface steps, and the reaction rate was significantly enhanced by 1) tailoring the catalytic activity through electrode surface impregnation with intrinsically catalytic nanoparticles and 2) electrochemical activation of surface species by imposing a net current through the electrode.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Universidad Politecnica de Valencia
Authors: Solis, C. (Ekstern), Navarrete, L. (Ekstern), Bozza, F. (Intern), Bonanos, N. (Intern), Serra, J. M. (Ekstern)
Pages: 1106-1110
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: ChemElectroChem
Volume: 2
ISSN (Print): 2196-0216
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 3.94 SJR 1.474 SNIP 0.727
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.77 SJR 1.501 SNIP 0.818
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.178 SNIP 0.648 CiteScore 3.13
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Chalcogenide compounds made by pulsed laser deposition at 355 and 248 nm

Thin films made by pulsed laser deposition may differ depending on the laser wavelength. We compared ZnS, Cu2SnS3 and a target enriched with SnS relative to Cu2SnS3 using 355 nm and 248 nm lasers.

General information
State: Published
Organisations: Department of Photonics Engineering, Optical Microsensors and Micromaterials, Department of Micro- and Nanotechnology, Silicon Microtechnology, DTU Danchip, Department of Energy Conversion and Storage, Electrofunctional materials, Technical University of Denmark
Authors: Ettlinger, R. B. (Intern), Cazzaniga, A. C. (Intern), Crovetto, A. (Intern), Ravnkilde, L. (Ekstern), Youngman, T. H. (Intern), Pryds, N. (Intern), Schou, J. (Intern)
Number of pages: 1
Publication date: 2015
Event: Poster session presented at 2015 E-MRS Spring Meeting, Lille, France.
Main Research Area: Technical/natural sciences
Electronic versions:
Poster_EMRS2015_Ettlingeretal_final.pdf

Bibliographical note
Poster presented at the EMRS Spring Meeting 2015 in Symposium CC: Laser and plasma processing for advanced applications in material science (poster CC.PI67, shown on May 11, 2015).
Source: PublicationPreSubmission
Source-ID: 118648818
Publication: Research - peer-review › Poster – Annual report year: 2015

Characterization of the contact between Bi2Te3-based materials and lead-free solder alloy under thermal cycling

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Authors: Van Nong, N. (Intern), Le, T. H. (Intern), Han, L. (Intern), Pham, H. N. (Intern), Pryds, N. (Intern)
Publication date: 2015

Host publication information
Title of host publication: Book of Abstracts - 34th Annual International Conference on Thermoelectrics (ICT 2015) and 13th European conference on Thermoelectrics (ECT 2015)
Article number: 15C.5
Main Research Area: Technical/natural sciences
Conference: 34th Annual International Conference on Thermoelectrics (ICT 2015) and 13th European conference on Thermoelectrics (ECT 2015), Dresden, Germany, 28/06/2015 - 28/06/2015
Electronic versions:
ITC2015_Book_of_Abstract_05.pdf
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2015

Charge Localization in the Lithium Iron Phosphate Li3Fe2(PO4)3 at High Voltages in Lithium-Ion Batteries

Possible changes in the oxidation state of the oxygen ion in the lithium iron phosphate Li3Fe2(PO4)3 at high voltages in lithium-ion (Li-ion) batteries are studied using experimental and computational analysis. Results obtained from synchrotron-based hard X-ray photoelectron spectroscopy and density functional theory (DFT) show that the oxidation state of O2− ions is altered to higher oxidation states (Oδ−, δ<2) upon charging Li3Fe2(PO4)3 to 4.7 V.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, Fundamental Electrochemistry
Authors: Younesi, R. (Intern), Christiansen, A. S. (Intern), Loftager, S. (Intern), García Lastra, J. M. (Intern), Vegge, T. (Intern), Norby, P. (Intern), Holtappels, P. (Intern)
Charge Transfer Induced Modulation Doping at Oxide Interfaces

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Authors: Chen, Y. (Intern)
Number of pages: 1
Publication date: 2015
Event: Abstract from Rare earth-transitional metal oxides and compounds for environment-friendly energy science and technology, Beijing, China.
Main Research Area: Technical/natural sciences
Electronic versions:
Charge_Transfer.pdf
Source: PublicationPreSubmission
Source-ID: 118749934
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2015

Charge transfer induced modulation doping of two-dimensional electron gas at complex oxide interfaces

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Authors: Chen, Y. (Intern), Trier, F. (Intern), Christensen, D. V. (Intern), Linderoth, S. (Intern), Pryds, N. (Intern)
Number of pages: 1
Publication date: 2015
Event: Abstract from TO-BE Spring Meeting 2015, Aveiro, Portugal.
Main Research Area: Technical/natural sciences
Electronic versions:
Charge_transfer_induced_modulation.pdf
Source: PublicationPreSubmission
Source-ID: 118749873
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2015

Colloidal stabilization of cerium-gadolinium oxide (CGO) suspensions via rheology

A rheological method based on the analysis of the flow index is proposed for the optimization of ceramic suspensions with respect to dispersant-ceramic affinity, dispersant concentration, and ceramic loading. The single-flow index (SFI) feature was identified as the criterion defining the optimized colloidal stable state. The method was applied to explore the ability of four commercial dispersants (acidic affine, neutral, basic affine, and polyvinylpyrrolidone (PVP)) to disperse cerium-gadolinium oxide (CGO) in ethanol. Only the acidic affine and the PVP dispersants were found to efficiently disperse the CGO powder. The acidic affine dispersant was further demonstrated to impart superior packing properties due to the formation of a thinner monolayer around the ceramic surface. CGO suspensions using the acidic affine at optimized amount were prepared and processed via tape casting. The resulting green tapes exhibited uniform and high packing density, producing a theoretical density in the sintered tapes of ca. 97-98%.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Imaging and Structural Analysis, Mixed Conductors
Authors: Marani, D. (Intern), Sudireddy, B. R. (Intern), Bentzen, J. J. (Intern), Jørgensen, P. S. (Intern), Kiebach, R. (Intern)
Pages: 2823–2832
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of the European Ceramic Society
Volume: 35
ISSN (Print): 0955-2219
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Ceramic suspensions, Cerium-gadolinium oxide, Colloidal stable state, Flow behavior, Rheology, Ceramic materials, Cerium, Elasticity, Gadolinium, Loading, Sintering, Cerium gadolinium oxide, Colloidal stabilization, Dispersant concentration, Flow behaviors, High packing density, Polyvinyl pyrrolidone, Stable state, Suspensions (fluids)

DOIs:
10.1016/j.jeurceramsoc.2015.03.043
Source: FindIt
Source-ID: 274686240
Publication: Research - peer-review › Journal article – Annual report year: 2015
Comparative Indoor and Outdoor Degradation of Organic Photovoltaic Cells via Inter-laboratory Collaboration

We report on the degradation of organic photovoltaic (OPV) cells in both indoor and outdoor environments. Eight different research groups contributed state of the art OPV cells to be studied at Pomona College. Power conversion efficiency, fill factor, and IV curves were collected at regular intervals over six to eight months. Similarly prepared devices were measured indoors, outdoors, and after dark storage. Device architectures are compared. Cells kept indoors performed better than outdoors due to the lack of temperature and humidity extremes. Encapsulated cells performed better due to the minimal oxidation. Some devices showed steady aging but many failed catastrophically due to corrosion of electrodes not active device layers. Degradation of cells kept in dark storage was minimal over periods up to one year.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Functional organic materials, Pomona College, Technische Universität Dresden, IMEC, Holst Center, Institut für Solarenergieforschung, Ilmenau University of Technology, Centre d’Investigación en Nanociencia i Nanotecnologia, Heliatek GmbH
Number of pages: 4
Pages: 1-4
Publication date: 2015

Host publication information
Title of host publication: Proceedings of 2015 IEEE 42nd Photovoltaic Specialist Conference (PVSC)
Publisher: IEEE
ISBN (Electronic): 978-1-4799-7944-8
Main Research Area: Technical/natural sciences
Conference: 42nd IEEE Photovoltaic Specialists Conference, New Orleans, United States, 14/06/2015 - 14/06/2015
DOIs: 10.1109/PVSC.2015.7356178
Source: FindIt
Source-ID: 276914242
Publication: Research - peer-review › Article in proceedings – Annual report year: 2015

Comparing superconducting and permanent magnets for magnetic refrigeration

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Authors: Bjørk, R. (Intern), Nielsen, K. K. (Intern), Bahl, C. R. (Intern), Smith, A. (Intern), Wulff, A. C. (Intern)
Number of pages: 1
Publication date: 2015

Host publication information
Title of host publication: Book of Abstracts. DTU's Sustain Conference 2015
Place of publication: Lyngby
Publisher: Technical University of Denmark (DTU)
Article number: E-7
Main Research Area: Technical/natural sciences
Conference: DTU Sustain Conference 2015, Lyngby, Denmark, 17/12/2015 - 17/12/2015
Electronic versions: E7_DTU_Sustain_2015.pdf
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2015

Comparison of direct and indirect plasma oxidation of NO combined with oxidation by catalyst
Direct and indirect plasma oxidation of NOx was tested in a medium-scale test-bench at gas flows of 50 slm (3 m³/h). For direct plasma oxidation the synthetic flue gas was directed through a stacked DBD reactor. For indirect plasma oxidation, a DBD reactor was used to generate ozone from pure O₂ and the plasma treated gas including ozone was mixed with flue gas at the entrance of a 6 m long serpentine-like reaction chamber which allowed reaction times longer than 10 s. At relatively low NOx concentrations of 200 ppm, both oxidation methods gave similar results. However, the temperature increase of the DBD reactor decreased the long-term efficiency of direct plasma oxidation. At the same time, the efficiency of indirect oxidation increased at elevated reactor temperatures. Additional experiments were carried out to
investigate the improvement of indirect oxidation by the introduction of catalyst to the reaction zone. Small-scale experiments with TiO2 powder demonstrated considerable efficiency gain for NOx oxidation while in medium-scale experiments, the efficiency improvement remained negligible. (c) 2014 Elsevier Ltd. All rights reserved.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, University of Tartu, Leibniz Institute for Plasma Science and Technology, West-Pomeranian Technical University, Lappeenranta University of Technology
Authors: Jogi, I. (Ekstern), Stamate, E. (Intern), Irimiea, C. (Intern), Schmidt, M. (Ekstern), Brandenburg, R. (Ekstern), Holub, M. (Ekstern), Bonislawski, M. (Ekstern), Jakubowski, T. (Ekstern), Kaariainen, M. (Ekstern), Cameron, D. C. (Ekstern)
Number of pages: 8
Pages: 137-144
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Fuel
Volume: 144
ISSN (Print): 0016-2361
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 5.4 SJR 1.891 SNIP 2.127
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.9 SJR 1.736 SNIP 2.207
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.781 SNIP 2.123 CiteScore 4.46
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.634 SNIP 2.294 CiteScore 4.14
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.762 SNIP 2.544 CiteScore 4.31
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.813 SNIP 2.425 CiteScore 3.99
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 2.041 SNIP 2.423 CiteScore 4.1
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.957 SNIP 2.298
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.985 SNIP 2.27
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.613 SNIP 2.156
Web of Science (2008): Indexed yes
Comparison Study of YBa$_2$Cu$_3$O$_{7-x}$ Films Deposited by Using Various Carboxylate Solutions

In this work, four fluorine-free solutions based on various carboxylates (propionates, butyrates, valerates, and hexanoates, respectively) were prepared and used for deposition of YBCO films on LaAlO$_3$ single-crystal substrates, in order to further understand the role of precursors on properties of the final films. After the same pyrolysis and sintering processes, the films from propionates and butyrates show pure YBCO phase and were epitaxially grown, as determined by X-ray diffractometer analysis. There are clear differences in morphologies of these four films, i.e., the films from propionates and butyrates exhibit platelike grains without distinct grain boundaries, while almost randomly orientated grains were observed on the surface of the other two films. As a result, we noticed significant discrepancies on their superconducting performance. The films from propionates and butyrates give Jc values (at 77 K, self-field) of 2.1 MA/cm$^2$ and 1.3 MA/cm$^2$, respectively, while no superconducting transition above 70 K was observed in the other two films. A relatively larger amount of carbonaceous residue left as a by-product after decomposition of carboxylates with longer ligands, particularly under fast pyrolysis and sintering processes, could be one of the explanations of the poor superconductivity in the films from the valerate and hexanoate-based precursors.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Atomic scale modelling and materials, Universidad Autonoma de Barcelona
Authors: Yue, Z. (Intern), Torres, P. (Ekstern), Norby, P. (Intern), Wulff, A. C. (Intern), Grivel, J. (Intern)
Number of pages: 4
Pages: 6600204
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: IEEE Transactions on Applied Superconductivity
Volume: 25
Issue number: 3
ISSN (Print): 1051-8223
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 1.45 SJR 0.408 SNIP 0.962
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.42 SJR 0.398 SNIP 1.145
Web of Science (2016): Indexed yes
Complete relaxation of residual stresses during reduction of solid oxide fuel cells
To assess the reliability of solid oxide fuel cell (SOFC) stacks during operation, the stress field in the stack must be known. During operation the stress field will depend on time as creep processes relax stresses. This work reports further details on a newly discovered creep phenomenon, accelerated creep, taking place during the reduction of the anode. This relaxes stresses at a much higher rate ($\times10^4$) than creep during operation. The phenomenon has previously been studied by simultaneous loading and reduction. With the recorded high creep rates, the stresses at the time of reduction should reduce significantly over minutes. In this work the stresses are measured in-situ before and after the reduction by use of XRD. The phenomenon of accelerated creep has to be considered both in the production of stacks and in the analysis of the stress field in a stack based on anode supported SOFCs.
Computational Analysis and Design of New Materials for Metal-Air Batteries

In the last decade, great effort has been paid to the development of next generation batteries. Metal-O2/Air batteries (Li-, Na-, Mg-, Al-, Fe- and Zn-O2 batteries) in both aqueous and nonaqueous (aprotic) electrolytes have gained much attention. Metal-air batteries have high theoretical specific gravimetric energy. In the case of Li-O2, it is comparable to that of gasoline. Thus, Li-O2 batteries could be attractive for electric vehicle manufacturers since the energy storage capacity accessible by commercially available Li-ion technology is too low to solve increasing capacity demands. However, current Li-O2 batteries suffer from several drawbacks, e.g. dendrite formation, poor rechargeability and low capacity caused by the so-called "sudden death" at its cathode during the discharge process due to insulating discharge products. This thesis is devoted to understand the charge transport in the main reaction products of emerging nonaqueous Li- and Na-O2 batteries at the atomistic level using the Density Functional Theory (DFT) method to address the latter problem. The role of cathode-electrolyte interface on charge transport and the implication of impurities from the air, particularly the effect of CO2 poisoning, in the performance of the battery are addressed. The present work involves computational investigations of different charge transport mechanisms, i.e. ionic, coherent electron, and polaronic transport. In order to validate the outcome from DFT calculations, results are compared with relevant experiments and show a notable agreement. The results of charge transport calculations in bulk Li2O2 (main discharge product in Li-O2 batteries) revealed that though it is a wide bandgap insulator (4.96 eV) it could offer fast ionic conduction with an activation barrier of 0.40 eV. Similarly, an accessible energy barrier for sodium ion diffusion is obtained in Na2O2 and in NaO2 (main discharge products in Na-O2 batteries). The transport mechanisms at the cathode-electrolyte interfaces, i.e. Li2O2@Li2CO3 interface, are also examined. Lithium vacancies accumulate at the peroxide side of this interface, reducing the coherent electron transport by two to three orders of magnitude compared to bulk pristine Li2O2. In contrast, the Li2O2@Li2CO3 interface shows an improved ionic conduction. For polaronic transport significant differences are also found in these two scenarios. In bulk Li2O2 the polaronic transport at room temperature is restricted to hole polarons, whereas electron polarons display very high hopping barriers (> 1.0 eV). By contrast, it is possible to have good mobilities for electron polarons at the Li2O2@Li2CO3 interface. Finally, our studies on the reaction mechanism of Li2O2 revealed that the CO2 poisoning, even at low concentrations of CO2 effectively blocks the step nucleation site and remarkably increases overpotentials and decreases the capacity of the battery.
Computationally Efficient Model of An Active Magnetocaloric Regenerator

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, University of Southern Denmark
Authors: Tahavori, M. (Ekstern), Veje, C. (Ekstern), Lei, T. (Intern), Nielsen, K. K. (Intern), Engelbrecht, K. (Intern)
Number of pages: 5
Publication date: 2015

Host publication information
Title of host publication: Proceedings of the 5th IEEE International Conference on Control Systems, Computing and Engineering
Publisher: IEEE
Main Research Area: Technical/natural sciences
Source: FindIt
Source-ID: 2287342363
Publication: Research - peer-review › Article in proceedings – Annual report year: 2015

Computational thermodynamics in electric current metallurgy
A priori derivation for the extra free energy caused by the passing electric current in metal is presented. The analytical expression and its discrete format in support of the numerical calculation of thermodynamics in electric current metallurgy have been developed. This enables the calculation of electric current distribution, current induced temperature distribution and free energy sequence of various phase transitions in multiphase materials. The work is particularly suitable for the study of magnetic materials that contain various magnetic phases. The latter has not been considered in literature. The method has been validated against the analytical solution of current distribution and experimental observation of microstructure evolution. It provides a basis for the design, prediction and implementation of the electric current metallurgy. The applicability of the theory is discussed in the derivations.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, The Open University
Authors: Bhowmik, A. (Intern), Qin, R. (Ekstern)
Pages: 1560-1563
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Materials Science and Technology
Volume: 31
Issue number: 13a
ISSN (Print): 0267-0836
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 1.89 SJR 0.889 SNIP 1.004
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.43 SJR 0.833 SNIP 0.859
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.623 SNIP 0.774 CiteScore 1.1
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.775 SNIP 0.996 CiteScore 1.1
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.631 SNIP 0.846 CiteScore 0.92
Computation of Effective Steady-State Creep of Porous Ni–YSZ Composites with Reconstructed Microstructures

This paper investigates the effective steady-state creep response of porous Ni–YSZ composites used in solid oxide fuel cell applications by numerical homogenization based on three-dimensional microstructural reconstructions and steadystate creep properties of the constituent phases. The Ni phase is found to carry insignificant stress in the composite and has a negligible role in the effective creep behavior. Thus, when determining effective creep, porous Ni–YSZ composites can be regarded as porous YSZ in which the Ni phase is counted as additional porosity. The stress exponents of porous YSZ are the same as that of dense YSZ, but the effective creep rate increases by a factor of 8–10 due to porosity. The relationship of creep rate and volume fraction of YSZ computed by numerical homogenization is underestimated by most existing analytical models. The Ramakrishnan–Arunchalam creep model provides the closest approximation among all analytical models.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Imaging and Structural Analysis
Authors: Kwok, K. (Intern), Jørgensen, P. S. (Intern), Frandsen, H. L. (Intern)
Pages: 2873–2880
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of the American Ceramic Society
Volume: 98
Issue number: 9
ISSN (Print): 0002-7820
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 1.325 SJR 0.95 CiteScore 3.06
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.77 SJR 1.028 SNIP 1.428
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.995 SNIP 1.37 CiteScore 2.71
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.167 SNIP 1.595 CiteScore 2.78
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.16 SNIP 1.48 CiteScore 2.52
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.271 SNIP 1.5 CiteScore 2.39
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.958 SNIP 1.447 CiteScore 2.45
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.449 SNIP 1.528
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.542 SNIP 1.43
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.433 SNIP 1.448
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.255 SNIP 1.444
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.128 SNIP 1.45
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.211 SNIP 1.614
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.592 SNIP 1.767
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.952 SNIP 1.816
Scopus rating (2002): SJR 2.021 SNIP 1.955
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 2.324 SNIP 2.38
Web of Science (2001): Indexed yes
Controlling the Activity and Stability of Pt-Based Electrocatalysts By Means of the Lanthanide Contraction

In order to reduce the Pt loading at the cathode of proton exchange membrane fuel cells (PEMFCs) more active and stable catalysts are needed to drive the oxygen reduction reaction. Most research has focussed on achieving this by alloying Pt with Fe, Co, Ni or Cu [1,2]. However, these compounds typically degrade under PEMFC conditions, due to dealloying. Alloys of Pt and lanthanides may be inherently less prone to dealloying under reactions conditions, due to their negative enthalpy of formation [2-4].

Herein we present a systematic study on the trends in activity of seven novel Pt-lanthanide electrodes (Pt5La, Pt5Ce, Pt5Sm, Pt5Gd, Pt5Tb, Pt5Dy and Pt5Tm). The materials are highly active, presenting a 3 to 6-fold activity enhancement over Pt [3-5], amongst the most active polycrystalline Pt-based catalyst ever reported. Moreover, our recent study showed that PtxGd is highly active in the nanoparticulate form [6]. On the bulk alloys, a Pt overlayer with a thickness of few Pt layers is formed onto the bulk alloys by acid leaching (Fig. 1A) [3-5]. The ORR activity versus the lattice parameter obtained by X-ray diffraction measurements follows a volcano relationship (Fig. 1B). Furthermore, we explain the trends in stability, and present the lattice parameter as a new descriptor that controls both the activity and stability of these materials. Using the lanthanide contraction we demonstrate that the electrocatalytic performance can be engineered by tuning the Pt-Pt distance.

CO2 Fixation by Membrane Separated NaCl Electrolysis

Atmospheric concentrations of carbon dioxide (CO2), a major cause of global warming, have been rising due to industrial development. Carbon capture and storage (CCS), which is regarded as the most effective way to reduce such atmospheric CO2 concentrations, has several environmental and technical disadvantages. Carbon capture and utilization (CCU), which has been introduced to cover such disadvantages, makes it possible to capture CO2, recycling byproducts as resources. However, CCU also requires large amounts of energy in order to induce reactions. Among existing CCU technologies, the process for converting CO2 into CaCO3 requires high temperature and high pressure as reaction conditions. This study proposes a method to fixate CaCO3 stably by using relatively less energy than existing methods. After forming NaOH absorbent solution through electrolysis of NaCl in seawater, CaCO3 was precipitated at room temperature and pressure. Following the experiment, the resulting product CaCO3 was analyzed with Fourier transform infrared spectroscopy (FT-IR); field emission scanning electron microscopy (FE-SEM) image and X-ray diffraction (XRD) patterns were also analyzed. The results showed that the CaCO3 crystal product was high-purity calcite. The study shows a successful method for fixating CO2 by reducing carbon dioxide released into the atmosphere while forming high-purity CaCO3.
Creation of High Mobility Two-Dimensional Electron Gases via Strain Induced Polarization at an Otherwise Nonpolar Complex Oxide Interface

The discovery of two-dimensional electron gases (2DEGs) in SrTiO$_3$-based heterostructures provides new opportunities for nanoelectronics. Herein, we create a new type of oxide 2DEG by the epitaxial-strain-induced polarization at an otherwise nonpolar perovskite-type interface of CaZrO$_3$/SrTiO$_3$. Remarkably, this heterointerface is atomically sharp and exhibits a high electron mobility exceeding 60 000 cm$^2$ V$^{-1}$ s$^{-1}$ at low temperatures. The 2DEG carrier density exhibits a critical dependence on the film thickness, in good agreement with the polarization induced 2DEG scheme.
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Center for Electron Nanoscopy, Imaging and Structural Analysis, Atomic scale modelling and materials, University of Copenhagen


Pages: 1849–1854
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Nano Letters
Volume: 15
Issue number: 3
ISSN (Print): 1530-6984

Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 13.07
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 13.4
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 14.76
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 14.04
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 14.23
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 13.78
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 13.83
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Web of Science (2008): Indexed yes
Web of Science (2007): Indexed yes
Web of Science (2006): Indexed yes
Web of Science (2005): Indexed yes
Web of Science (2003): Indexed yes
Web of Science (2002): Indexed yes
Web of Science (2001): Indexed yes

Original language: English
Complex oxide interfaces, Oxide electronics, Two-dimensional electron gases, Strain induced polarization

DOIs:
10.1021/nl504622w
CsH$_2$PO$_4$/NdPO$_4$ Composites as Proton Conducting Electrolytes for Intermediate Temperature Fuel Cells

Composite proton conducting materials based on cesium dihydrogen phosphate and neodymium phosphate hydrate were prepared and investigated in terms of X-ray diffraction, thermogravimetry, conductivity, stability and fuel cell performance. At 150°C the conductivity was $1.8 \times 10^{-6}$ S cm$^{-1}$ for the pristine cesium dihydrogen phosphate and $0.8 \times 10^{-4}$ S cm$^{-1}$ for neodymium phosphate hydrate, while that of the composite containing 29 mol% neodymium phosphate and 71 mol% cesium dihydrogen phosphate was $0.4 \times 10^{-2}$ S cm$^{-1}$. It was proposed that the interaction between the two components establishes a dynamic hydrogen bonding network enabling efficient proton conduction long before the development of the extensive phase disordering of the superprotonic transition. The presence of thermally stable hydrate water present in neodymium phosphate may also play a role in improving both conductivity and stability of the solid acid. The electromotive force, open circuit voltage and fuel cell performance were measured as demonstration of the material application.
Degradation Studies on LiFePO$_4$ cathode

In this paper we examine a laboratory LiFePO$_4$ (LFP) cathode and propose a simple model that predicts the electrode capacity as function of C-rate, number of cycles and calendar time. Microcracks were found in Li$_{1-x}$FePO$_4$ particles in a degraded LFP electrode and low-acceleration voltage (1 kV) FIB/SEM analysis allowed us to obtain phase contrast between FePO$_4$ and LiFePO$_4$. The evolution of micro-cracks is expected to increase the concentration of LFP particles which are not electronically accessible and thus cause a loss in capacity.
Depth profiling the solid electrolyte interphase on lithium titanate (Li4Ti5O12) using synchrotron-based photoelectron spectroscopy

The presence of a surface layer on lithium titanate (Li4Ti5O12, LTO) anodes, which has been a topic of debate in scientific literature, is here investigated with tunable high surface sensitive synchrotron-based photoelectron spectroscopy (PES) to obtain a reliable depth profile of the interphase. Li||LTO cells with electrolytes consisting of 1 M lithium hexafluorophosphate dissolved in ethylene carbonate:diethyl carbonate (LiPF6 in EC:DEC) were cycled in two different voltage windows of 1.0-2.0 V and 1.4-2.0 V. LTO electrodes were characterized after 5 and 100 cycles. Also the pristine electrode as such, and an electrode soaked in the electrolyte were analyzed by varying the photon energies enabling depth profiling of the outermost surface layer. The main components of the surface layer were found to be ethers, P-O containing compounds, and lithium fluoride.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, Uppsala University
Authors: Nordh, T. (Ekstern), Younesi, R. (Intern), Brandell, D. (Ekstern), Edström, K. (Ekstern)
Number of pages: 7
Pages: 173-179
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Power Sources
Volume: 294
ISSN (Print): 0378-7753
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 7 SJR 2.202 SNIP 1.536
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 6.22 SJR 1.944 SNIP 1.5
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.9 SNIP 1.667 CiteScore 6.34
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.964 SNIP 2.042 CiteScore 6.3
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.975 SNIP 2.137 CiteScore 5.63
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.282 SNIP 2.006 CiteScore 5.04
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.227 SNIP 2.172 CiteScore 5.13
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 2.294 SNIP 1.972
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 2.105 SNIP 1.785
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.96 SNIP 1.713
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.587 SNIP 1.488
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.802 SNIP 2.223
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.656 SNIP 1.809
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.85 SNIP 1.805
Scopus rating (2003): SJR 1.66 SNIP 1.57
Scopus rating (2002): SJR 2.385 SNIP 1.409
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 1.146 SNIP 1.506
Scopus rating (2000): SJR 0.649 SNIP 0.949
Scopus rating (1999): SJR 0.814 SNIP 0.988
Original language: English
Li-ion batteries, LTO, PES, SEI, Surface layer, XPS, Depth profiling, Electrodes, Electrolytes, Ethylene, Lithium, Lithium compounds, Photoelectron spectroscopy, Photoelectrons, Photons, Solid electrolytes, Titanium compounds, X ray photoelectron spectroscopy, Surface layers, Lithium-ion batteries
DOIs:
10.1016/j.jpowsour.2015.06.038
Source: FindIt
Source-ID: 275297209
Publication: Research - peer-review › Journal article – Annual report year: 2015
Design and experimental tests of a rotary active magnetic regenerator prototype

A rotary active magnetic regenerator (AMR) prototype with efficiency and compact design as focus points has been designed and built. The main objective is to demonstrate improved efficiency for rotary devices by reducing heat leaks from the environment and parasitic mechanical work losses while optimizing the utilization of the magnetized volume. Heat transfer calculations combined with 1D AMR modeling have revealed the necessity for an insulating air gap between magnet and regenerator when designing for high efficiency. 2D finite difference AMR modeling capturing the interplay between heat transfer fluid flow and an inhomogenous time-varying magnetic field in the individual regenerator beds has been used in the design process. For one operating point a COP of 3.1 at a temperature span of 10.2 K and a cooling power of 103 W were measured. Major issues limiting the performance have been identified and improvements are outlined for future work. © 2015 Elsevier Ltd and IIR. All rights reserved.
Design and Optimization of Effective Segmented Thermoelectric Generator for Waste Heat Recovery

Energy safety is a vital issue of the global future. Together with developing renewable and eco-friendly energy sources, recovering waste energy is no less of an important issue. It is estimated that 60% of energy converted in most of today's energy processes nowadays is waste, mainly in the form of heat. Using thermoelectric generators, which convert heat into electricity, is a promising way to recover waste energy. However, the efficiency of thermal-to-electricity converters needs to be improved in order to be widely applied in practice. Despite the fact that significant amount of efforts have been focused on material development, realizing high efficient thermoelectric generators from such well-developed materials is still limited. Moreover, no single thermoelectric material could withstand the wide temperature range required to boost efficiency of TEGs. By segmentation of different TE materials which operate optimally in each temperature range, this study aims at developing high performance segmented TEGs for medium-high (450 – 850 K) temperature application. The research is focused on the challenges in joining and minimizing the contact resistances between different TE materials and with metal electrode.

One-dimensional numerical modeling was employed to design and predict the efficiency of segmented materials built up from most of today's state-of-the-art thermoelectric materials. Combinations of materials that would deliver the highest conversion efficiency in different temperature ranges of 300 – 700, and 900 – 1100 K are considered. The obtained results reveals that segmented thermoelectric generator comprising of Bi0.6Sb1.4Te3/Ba8Au5.3Ge40.7/PbTe-SrTe/SiGe as p-leg and either segmented Bi2Te3/PbTe/SiGe or Bi2Te3/Ba0.08La0.05Yb0.04Co4Sb12/La3Te4 as n-leg working in 300 – 1100 K temperature range could achieve a maximum efficiency of 18.2 %. In lower working temperature ranges of 300 – 700 and 300 – 900 K, the maximum efficiencies are 13.5 and 16.6 %, respectively for segmented TEGs of p-legBi0.6Sb1.4Te3/TAGS ((AgSbTe)0.15(GeTe)0.85) with n-leg Bi2Te3/PbTe and p-leg Bi0.6Sb1.4Te3/Ba8Au5.3Ge40.7/PbTe-SrTe with n-leg Bi2Te3/PbTe/SiGe. The results could provide a guideline to develop high efficiency segmented thermoelectric generators. Based on these theoretical results, segmentation of half-Heusler alloys and Bi2Te3 materials was selected for further study.

Firstly, the joining between thermoelectric p- and n-type half-Heusler (HH) alloys and silver electrode at hot side was developed. A fast-hot pressing method was introduced to directly join the HH materials with silver interconnecting layer. The method was also compared with the conventional joining method where a third material is used as filler. Microstructures and interfacial chemical evolution at the joining interfaces were investigated using scanning electron microscopy (SEM) and energy dispersive spectroscopy (EDS). The transport properties of the joint, including thermopower across the interfaces and contact resistance as a function of temperature were studied. With fast hot pressing method, the contact resistance between HH alloys and Ag-electrode could be significantly reduced by about 50 %. Moreover, by avoiding a third filler material, the method limits the formation of new phases at contact interface which might degrade the overall thermoelectric properties. This work is a crucial step to make segmented HH/BiTe TEG.

Then, p- and n- type segmented legs of bismuth tellurides and half-Heusler alloys were built and characterized. Segmentation of bismuth tellurides to half-Heusler/Ag was processed at temperature 493 K, pressure 30 MPa in vacuum using Ag10Sn90 solder as filler. Interface microstructural evolution and thermoelectric properties of segmented legs were then investigated. The contact resistance of the joint parts as a function of temperature was measured from room temperature to 473 K. Numerical modeling was used to evaluate the influence of measured contact resistances on the final power generating properties of the obtained segmented legs and their unicouple. Under working temperature from 323 to 873 K, the obtained p-segmented legs could deliver a power density of 0.3 Wcm-2 and maximum voltage of 115 mV. With the same condition, the power density and maximum voltage generated by n-segmented leg were 0.25 Wcm-2 and 102 mV. These values are significantly smaller than calculation data. The reason is possibly due to the contact between BiTe and electrode at the cold end, thus improvement of the cold side contact was made. At temperature gradient of 498 K, the maximum power density of the improved n-segmented leg was 0.8 Wcm-2, giving a maximum efficiency of 4.5%.
Design of two-photon molecular tandem architectures for solar cells by ab initio theory
An extensive database of spectroscopic properties of molecules from ab initio calculations is used to design molecular complexes for use in tandem solar cells that convert two photons into a single electron–hole pair, thereby increasing the output voltage while covering a wider spectral range. Three different architectures are considered: the first two involve a complex consisting of two dye molecules with appropriately matched frontier orbitals, connected by a molecular diode. Optimized combinations of dye molecules are determined by taking advantage of our computational database of the structural and energetic properties of several thousand porphyrin dyes. The third design is a molecular analogy of the intermediate band solar cell, and involves a single dye molecule with strong intersystem crossing to ensure a long lifetime of the intermediate state. Based on the calculated energy levels and molecular orbitals, energy diagrams are presented for the individual steps in the operation of such tandem solar cells. We find that theoretical open circuit voltages of up to 1.8 V can be achieved using these tandem designs. Questions about the practical implementation of prototypical devices, such as the synthesis of the tandem molecules and potential loss mechanisms, are addressed.
Development and Manufacture of Polymer-based Electrochromic Devices

The field of organic electrochromics is reviewed here, with particular focus on how the "electrochromic" as a functional material can be brought from the current level of accurate laboratory synthesis and characterization to the device and application level through a number of suited roll-to-roll methods compatible with upscaling and manufacture. The successful approaches to operational devices are presented in detail, as well as areas where future research would have a high impact and accelerate the development such as highly conducting and transparent substrates, electrolytes adapted for multilayer application and morphologically stable conjugated polymers.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Functional organic materials, Clayton State University
Authors: Jensen, J. (Intern), Hösel, M. (Intern), Dyer, A. L. (Ekstern), Krebs, F. C. (Intern)
Pages: 2073–2090
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Advanced Functional Materials
Volume: 25
Issue number: 14
ISSN (Print): 1616-301X
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 12.51
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 11.56
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 11.93
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 11.32
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 10.6
ISI indexed (2013): ISI indexed yes
Development of ceramic multilayer devices for clean and efficient energy conversion

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Mixed Conductors
Authors: Kaiser, A. (Intern), Gurauskis, J. (Intern), Cheng, S. (Intern), Hendriksen, P. V. (Intern)
Number of pages: 2
Publication date: 2015

Host publication information
Title of host publication: Proceedings of the 14th International Conference on Environmental Science and Technology, CEST2015
Article number: CEST2015-00193
ISBN (Print): 978-960-7475-52-7
Main Research Area: Technical/natural sciences
Conference: 14th International Conference on Environmental Science and Technology, Rhodes, Greece, 03/09/2015 - 03/09/2015
Electronic versions:
CEST2015_00193_A_Kaiser_Extended_Abstract
Source: PublicationPreSubmission
Source-ID: 106310650
Publication: Research - peer-review › Journal article – Annual report year: 2015

Development of high temperature PEM fuel cells. Simplification and CO tolerance mapping

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors
Authors: Jensen, J. O. (Intern), Fernandez, S. M. (Intern), Vassiliev, A. (Intern), Cleemann, L. N. (Intern), Li, Q. (Intern)
Number of pages: 27
Publication date: 2015

Publication information
Media of output: PowerPoint
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
Presentation

Bibliographical note
We describe and review how the scaling of printed energy technologies not only requires scaling of the input materials but also the machinery used in the processes. The general consensus that ultrafast processing of technologies with large energy capacity can only be realized using roll-to-roll methods is taken as a premise, and thus the progression from a highly successful laboratory technique (i.e., spin coating) to large-scale roll-to-roll equipment is described in terms of all of the intermediate steps that must be available to make the transfer possible. Spin coating is compatible with materials availability on the small scale and efficient scaling of equipment is a demanding task that must be performed in parallel with increasing materials availability. We outline that 3–5 processing platforms are necessary to efficiently take the laboratory technology to a version that represents the lower end of the industrial scale. The machinery bridges the gap through firstly achieving improved ink efficiency without surface contact, followed by better ink efficiency at higher speeds, and finally large-area processing at high speed with very high ink efficiency.
demonstrate our method using two data sets from material science – a phantom data set of a solid oxide fuel cell simulation for detecting three phases and their interfaces, and a tomogram of a glass fiber composite used in wind turbine blades for detecting individual glass fibers.

**General information**
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Image Analysis & Computer Graphics, Department of Wind Energy, Composites and Materials Mechanics, Department of Energy Conversion and Storage, Imaging and Structural Analysis
Number of pages: 12
Pages: 504-515
Publication date: 2015

**Host publication information**
Title of host publication: Image Analysis : 19th Scandinavian Conference, SCIA 2015 Copenhagen, Denmark, June 15–17, 2015 Proceedings
Publisher: Springer Science+Business Media
ISBN (Print): 978-3-319-19664-0
ISBN (Electronic): 978-3-319-19665-7

Series: Lecture Notes in Computer Science
ISSN: 0302-9743
BFI conference series: Scandinavian Conference on Image Analysis (5010789)
Main Research Area: Technical/natural sciences
Conference: 19th Scandinavian Conference on Image Analysis, Copenhagen, Denmark, 15/06/2015 - 15/06/2015
Volume segmentation, Materials images, X-ray tomography, Learning dictionaries, Glass fiber segmentation
Electronic versions:
DOIs:
10.1007/978-3-319-19665-7_43

**Relations**
Projects:
Dictionary Based Segmentation in Volumes
Publication: Research - peer-review › Article in proceedings – Annual report year: 2015

**Dictionary Based Segmentation in Volumes**
Method for supervised segmentation of volumetric data. The method is trained from manual annotations, and these annotations make the method very flexible, which we demonstrate in our experiments. Our method infers label information locally by matching the pattern in a neighborhood around a voxel to a dictionary, and hereby accounts for the volume texture.

**General information**
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Image Analysis & Computer Graphics, Department of Wind Energy, Composites and Materials Mechanics, Department of Energy Conversion and Storage, Imaging and Structural Analysis
Number of pages: 1
Publication date: 2015
Event: Poster session presented at 19th Scandinavian Conference on Image Analysis, Copenhagen, Denmark.
Main Research Area: Technical/natural sciences
Electronic versions:
posterSCIA.pdf

**Bibliographical note**
This poster is connected with the article in proceeding: R.R. Paulsen and K.S. Pedersen (Eds.): SCIA 2015, LNCS 9127, pp. 504–515, 2015. DOI: 10.1007/978-3-319-19665-7_43
Publication: Research - peer-review › Poster – Annual report year: 2016
Direct Coal Oxidation in Modified Solid Oxide Fuel Cells

Hybrid direct carbon fuel cells employ a classical solid oxide fuel cell together with carbon dispersed in a carbonate melt on the anode side. In a European project, the utilization of various coals has been investigated with and without addition of an oxidation catalyst to the carbon-carbonate slurry or anode layer. The nature of the coal affects both open circuit voltage and power output. Highest OCV and power densities were observed for bituminous coal and by adding manganese oxide or praseodymium-doped ceria to the carbon/carbonate mixture. Comparing the carbon black fueled performance of an anode supported (315 µm anodes) and cathode supported cell (15 µm anode) indicates a superior performance of the latter. Using uncatalyzed biomass (charcoal) as fuel results in an OCV of 941 mV and a maximum power density of 78 mW/cm² at 755°C similar to the power output of manganese oxide catalyzed bituminous coal (73 mW/cm²).

© 2015 ECS - The Electrochemical Society

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Fundamental Electrochemistry, Centro Nacional del Hidrogeno
Authors: Deleebeeck, L. (Intern), Gil, V. (Intern), Ippolito, D. (Intern), Campana, R. (Ekstern), Kammer Hansen, K. (Intern) , Holtappels, P. (Intern)
Pages: 2685-2694
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: E C S Transactions
Volume: 68
Issue number: 1
ISSN (Print): 1938-5862
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 0.44 SJR 0.225 SNIP 0.252
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 0.4 SJR 0.228 SNIP 0.253
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.211 SNIP 0.244 CiteScore 0.36
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.212 SNIP 0.234 CiteScore 0.36
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.192 SNIP 0.231 CiteScore 0.27
ISI indexed (2013): ISI indexed no
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.241 SNIP 0.26 CiteScore 0.29
ISI indexed (2012): ISI indexed no
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.261 SNIP 0.28 CiteScore 0.36
ISI indexed (2011): ISI indexed no
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.249 SNIP 0.251
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.242 SNIP 0.27
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.254 SNIP 0.255
Scopus rating (2007): SJR 0.213 SNIP 0.206
Scopus rating (2006): SJR 0.134 SNIP 0.073
Original language: English
DOIs:
10.1149/06801.2685ecst
Direct measurements of the magnetic entropy change
An experimental device that can accurately measure the magnetic entropy change, $\Delta s$, as a function of temperature, $T$, and magnetic field, $H$, is presented. The magnetic field source is in this case a set of counter-rotating concentric Halbach-type magnets, which produce a highly homogeneous applied field with constant orientation. The field may be varied from 0 to 1.5 T in a continuous way. The temperature stability of the system is controlled to within $\pm 10$ mK and the standard range for the current setup is from 230 K to 330 K. The device is under high vacuum and we show that thermal losses to the ambient are negligible in terms of the calorimetric determination of the magnetic entropy change, while the losses cannot be ignored when correcting for the actual sample temperature. We apply the device to two different types of samples; one is commercial grade Gd, i.e., a pure second-order phase transition material, while the other is Gd$_5$Si$_2$Ge$_2$, a first order magnetic phase transition material. We demonstrate the device’s ability to fully capture the thermal hysteresis of the latter sample by following appropriate thermal resetting scheme and magnetic resetting scheme. © 2015 AIP Publishing LLC.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Number of pages: 6
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Review of Scientific Instruments
Volume: 86
Issue number: 10
Article number: 103903
ISSN (Print): 0034-6748
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 1.32 SJR 0.585 SNIP 0.858
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.2 SJR 0.703 SNIP 1.048
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.686 SNIP 0.908 CiteScore 1.11
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.972 SNIP 1.261 CiteScore 1.45
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.9 SNIP 1.099 CiteScore 1.28
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.017 SNIP 1.277 CiteScore 1.45
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.868 SNIP 1.108 CiteScore 1.43
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Dispenser printed thermoelectric generators

**General information**

State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Fraunhofer Institut für Werkstoff- und Strahltechnik, Dresden University of Technology
Authors: Stepien, L. (Ekstern), Roch, A. (Ekstern), Schlaier, S. (Ekstern), Abt, M. (Ekstern), Hoch, C. (Ekstern), Dani, I. (Ekstern), Van Nong, N. (Intern), Lukowicz, M. V. (Ekstern), Leyens, C. (Ekstern)
Publication date: 2015

**Host publication information**

Title of host publication: Book of Abstracts - 34th Annual International Conference on Thermoelectrics (ICT 2015) and 13th European conference on Thermoelectrics (ECT 2015)
Article number: 9C.2
Main Research Area: Technical/natural sciences
Conference: 34th Annual International Conference on Thermoelectrics (ICT 2015) and 13th European conference on Thermoelectrics (ECT 2015), Dresden, Germany, 28/06/2015 - 28/06/2015
Electronic versions:
ITC2015_Book_of_Abstract_08.pdf
Source: PublicationPreSubmission
Source-ID: 111973395
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2015

Durable thin ceramic films for improvement of Proton Exchange Membrane (PEM) electrolysis
Dynamic behavior of impurities and native components in model LSM microelectrodes on YSZ

Strontium-doped lanthanum manganese is a widely used cathode material in solid oxide fuel cells. Segregation phenomena can have a critical impact on performance and durability, especially when they cause active interfaces to degrade. The segregation behavior in polarized and non-polarized strontium-doped lanthanum manganese ((La0.75Sr0.25)0.95MnO3) microelectrodes with a diameter of 100 μm and a thickness of ~500 nm on an yttria-stabilized zirconia electrolyte were analyzed post-mortem after ~200 h at temperatures up to 850 °C. Time-of-flight secondary ion mass spectrometry was used to study the dynamic behavior of the native components (La, Sr, Mn) and selected impurities (Si, K, Na) both laterally and in-depth. Manganese was found to be especially mobile and showed both segregation onto the electrolyte as a result of temperature and polarization and dissolution into the electrolyte below the microelectrodes. All native components showed a complex in-depth dynamic behavior, and a nanoscale in-depth analysis of the electrode-electrolyte interface revealed the formation of a well-defined lanthanum zirconate layer. The selected impurities segregated to the electrolyte and microelectrode surfaces and Na- and K-rich layers formed at different depths.
Dynamic rotor mode in antiferromagnetic nanoparticles

We present experimental, numerical, and theoretical evidence for an unusual mode of antiferromagnetic dynamics in nanoparticles. Elastic neutron scattering experiments on 8-nm particles of hematite display a loss of diffraction intensity with temperature, the intensity vanishing around 150 K. However, the signal from inelastic neutron scattering remains above that temperature, indicating a magnetic system in constant motion. In addition, the precession frequency of the inelastic magnetic signal shows an increase above 100 K. Numerical Langevin simulations of spin dynamics reproduce all measured neutron data and reveal that thermally activated spin canting gives rise to an unusual type of coherent magnetic precession mode. This "rotor" mode can be seen as a high-temperature version of superparamagnetism and is driven by exchange interactions between the two magnetic sublattices. The frequency of the rotor mode behaves in fair agreement with a simple analytical model, based on a high-temperature approximation of the generally accepted Hamiltonian of the system. The extracted model parameters, such as the magnetic interaction and the axial anisotropy, are in excellent agreement with results from Mossbauer spectroscopy.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Electrofunctional materials, Imaging and Structural Analysis, University of Copenhagen, Research Center Jülich GmbH, Technical University of Denmark
Number of pages: 10
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Physical Review B Condensed Matter
Volume: 91
Issue number: 9
ISSN (Print): 0163-1829
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 3.34 SJR 1.604 SNIP 1.04
Web of Science (2017): Indexed yes
Scopus rating (2016): CiteScore 3.16 SJR 2.339 SNIP 1.151
Web of Science (2016): Indexed yes
Scopus rating (2015): SJR 2.377 SNIP 1.13 CiteScore 2.8
Web of Science (2015): Indexed yes
Scopus rating (2014): SJR 2.762 SNIP 1.316 CiteScore 3.3
Ecodesign of organic photovoltaic modules from Danish and Chinese perspectives

The life cycle of a solar park made using organic photovoltaic (OPV) technology is assessed here. The modules have been fabricated in a pilot scale plant and they have been installed together with other components to evaluate the balance of system, in a solar park located in Denmark. Three possible waste management practices have been contemplated for the end of life of the solar park: recycling, incineration or the average local mix. The assessment of the environmental impacts of such a system reveals that silver used in the electrodes is overall the largest source of impacts, such as chemical pollution and metal depletion. The establishment of resource recovery systems for the end-of-life management of the OPV modules is therefore crucial to reduce overall environmental impacts. Liability on the manufacturers or on the operators should be implemented. The electricity produced from OPV solar parks yields similar footprints to other traditional energy technologies; e.g. coal and natural gas. However, when the efficiency of the OPV modules is increased from 1% to 5% they are comparable to other mature PV technologies already on the market. The effects of outsourcing or exporting the production of the OPV modules from Denmark to China have additionally been studied to determine the most advantageous configuration. The stakeholders should aim at anchoring the manufacturing of solar parks in countries with stringent emission standards and/or high technology efficiencies, e.g. Denmark, and at deploying them in countries with high solar radiation to maximise the environmental benefits of the PV technology.
Economic Potential of Biomass from Unused Agriculture Land for Energy Use: Case of Croatia

In this paper the energy potential of biomass from growing short rotation coppice (SRC) on unused agricultural land in the Republic of Croatia was examined. At present, SRC is not completely recognized in Croatian legislative and considerations in energy strategy and action plans. The paper aspires to contribute to better understanding of the role SRC can take in national and local energy planning. The methodology is provided for regional analysis of biomass energy potential on unused agricultural land and for assessing the cost of the biomass at the power plant (PP) location considering transport distance, transport costs and size of the power plants up to 15 MWe, which was applied on the case of Croatian counties. Case studies have been analysed for optimal locations of such power plants depending on energy potential of SRC in various counties. Operation costs are also calculated for such power plants and appropriate size of
seasonal heat storage is discussed for each case study. Case studies have shown the potential for use of previously unused agricultural land to help achieve national targets for renewable energy sources as well as reducing carbon dioxide emissions, help diversify the landscape and increase biodiversity. Through scenario approach, technical and energy potential of SRC is investigated and noticeable potential in Karlovac and Sisak-Moslavina Counties, due to large area of unused agricultural land in those counties. Energy potential of those counties is 2.2 PJ/year for Karlovac and 1.7 PJ/year for Sisak-Moslavina Country. With price of biomass at gate of power plant in best scenario reaching 44.7 €/t, novel systems of combined cooling, heating and power generation (CCHP) are not yet feasible, but SRC could be considered in already established central district heating systems.

**General information**

State: Published


Authors: Pfeifer, A. (Ekstern), Dominkovic, D. F. (Intern), Ćosić, B. (Ekstern)

Pages: 351-351

Publication date: 2015

**Host publication information**

Title of host publication: Book of Abstracts : 10th Conference on Sustainable Development of Energy, Water and Environment Systems

Article number: SDEWES2014.0399

Main Research Area: Technical/natural sciences


Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2015

**Effectiveness of electronic stability control on single-vehicle accidents**

Objective: This study aims at evaluating the effectiveness of electronic stability control (ESC) on single-vehicle injury accidents while controlling for a number of confounders influencing the accident risk.

Methods: Using police-registered injury accidents from 2004 to 2011 in Denmark with cars manufactured in the period 1998 to 2011 and the principle of induced exposure, 2 measures of the effectiveness of ESC were calculated: The crude odds ratio and the adjusted odds ratio, the latter by means of logistic regression. The logistic regression controlled for a number of confounding factors, of which the following were significant. For the driver: Age, gender, driving experience, valid driving license, and seat belt use. For the vehicle: Year of registration, weight, and ESC. For the accident surroundings: Visibility, light, and ESC. For the road: Speed limit, surface, and section characteristics. Results: The present study calculated the crude odds ratio for ESC-equipped cars of getting in a single-vehicle injury accident as 0.40 (95% confidence interval [CI], 0.34-0.47) and the adjusted odds ratio as 0.69 (95% CI, 0.54-0.88). No difference was found in the effectiveness of ESC across the injury severity categories (slight, severe, and fatal). Conclusions: In line with previous results, this study concludes that ESC reduces the risk for single-vehicle injury accidents by 31% when controlling for various confounding factors related to the driver, the car, and the accident surroundings. Furthermore, it is concluded that it is important to control for human factors (at a minimum age and gender) in analyses where evaluations of this type are performed.

**General information**

State: Published

Organisations: Department of Transport, Traffic modelling and planning, Department of Energy Conversion and Storage, Imaging and Structural Analysis

Authors: Lyckegaard, A. (Intern), Hels, T. (Intern), Bernhoft, I. M. (Intern)

Pages: 380-386

Publication date: 2015

Main Research Area: Technical/natural sciences

**Publication information**

Journal: Traffic Injury Prevention

Volume: 16

Issue number: 4

ISSN (Print): 1538-9588

Ratings:

BFI (2018): BFI-level 1

Web of Science (2018): Indexed yes

BFI (2017): BFI-level 1

Scopus rating (2017): SNIP 1.065 SJR 0.773 CiteScore 1.4

Web of Science (2017): Indexed Yes

BFI (2016): BFI-level 1

Scopus rating (2016): CiteScore 1.45 SJR 0.735 SNIP 1.013
Effect of Aging on the Electrochemical Performance of LSM-YSZ Cathodes

Investigations of degradation mechanisms of solid oxide fuel cells are crucial for achieving a widespread commercialization of the technology. In this work, electrochemical impedance spectroscopy (EIS) was applied for studying the aging effect on LSM-YSZ cathodes exposed to humidified air at 900°C for up to 3000 h. EIS spectra were fitted by a transmission line model for estimating relevant parameters associated with the LSM/YSZ charge transfer reaction and the oxide ion conduction through the YSZ network. For the reference non-aged sample, the ionic conductivity values are the expected ones for YSZ with 1 eV activation energy and no dependency on oxygen partial pressure (pO2), while the charge transfer resistance presents an activation energy of 1.6 eV and is proportional to (pO2)−0.31±0.08. These values agree with those reported in literature, validating the used model. The charge transfer resistance shows no clear tendency with aging time, while the ionic conductivity decreases up to ∼79%. Accordingly, the electrochemically active thickness contracts from 60–135 μm to 45–60 μm. The changes observed in the cathode transport and electrochemical properties are mostly explained by the evolution of the phases present in agreement with results previously reported in the literature.
Effect of BaZrO3/Ag hybrid doping to the microstructure and performance of fluorine-free MOD method derived YBa2Cu3O7−x superconducting thin films

It is known that BaZrO3 and Ag can improve the magnetic and transport performance of YBCO thin film through totally disparate ways. BaZrO3 plays the role of flux pinning centers and Ag improves the transparency of the YBCO grain boundaries. However, similar research is rare on the fluorine-free derived YBCO films. In this research, BaZrO3-doped, Ag-doped and BaZrO3/Ag hybrid-doped YBCO films were synthesized through a fluorine-free metal–organic deposition method. BaZrO3 was found to deteriorate the microstructure and performance of YBCO, while Ag-doping was found to enhance the crystallization of YBCO and resulted in a high Jc of 3.87 MA/cm² in self-field at 77 K. However, the microstructure and performance of the BaZrO3/Ag hybrid-doped YBCO film showed that the positive impact of Ag-doping was totally overwhelmed by that of BaZrO3.
Effect of chemical redox on Gd-doped ceria mass diffusion

The valence and size of cations influence mass diffusion and oxygen defects in ceria. Here we show that reduction of Ce$^{4+}$ to Ce$^{3+}$, at high temperatures and low oxygen activity, activates fast diffusion mechanisms which depend on the aliovalent cation concentration. As a result, polycrystalline solid solutions with enhanced electrochemical properties are formed.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Ceramic Engineering & Science, Universidade Federal do ABC
Number of pages: 4
Pages: 18835-18838
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Materials Chemistry A
Volume: 3
Issue number: 37
ISSN (Print): 2050-7488
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 9.61 SJR 3.488 SNIP 1.55
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 8.46 SJR 3.075 SNIP 1.479
Effect of Co$_3$O$_4$ and Co$_3$O$_4$/CeO$_2$ infiltration on the catalytic and electro-catalytic activity of LSM$_{15}$/CGO$_{10}$ porous cell stacks for oxidation of propene

The objective of this work was to study the effect of Co3O4 and Co3O4/CeO2 infiltration on the propene oxidation catalytic activity of a La$_{0.85}$Sr$_{0.15}$MnO$_3$/Ce$_{0.9}$Gd$_{0.1}$O$_{1.95}$ electrochemical porous cell stack (11 layers, 5 single cells in series). The effect of the infiltration of Co$_3$O$_4$ and Co$_3$O$_4$/CeO$_2$ on the electrochemical properties of the porous cell stack was also investigated by electrochemical impedance spectroscopy (EIS). Co$_3$O$_4$ and Co$_3$O$_4$/CeO$_2$ exhibited high catalytic activity for propene oxidation. The increase of propene oxidation rate with +4 V (0.8 V/cell) polarization reached 10% for the Co$_3$O$_4$ infiltrated reactor and 48% of efficiency at 300 °C. The Co$_3$O$_4$/CeO$_2$ co-infiltration decreased the reactor polarization resistance, while Co$_3$O$_4$ infiltration had negligible effect on reactor electrochemical performance. The beneficial effect of CeO$_2$ on the electrode activity was attributed to the increased concentration of stable oxygen species on the electrode surface.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Fundamental Electrochemistry
Authors: Ippolito, D. (Intern), Kammer Hansen, K. (Intern)
Number of pages: 6
Pages: 23-28
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Electrochimica Acta
Volume: 159
ISSN (Print): 0013-4686
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 5.01 SJR 1.439 SNIP 1.101
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.74 SJR 1.355 SNIP 1.177
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.321 SNIP 1.324 CiteScore 4.86
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.378 SNIP 1.456 CiteScore 4.59
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.427 SNIP 1.587 CiteScore 4.44
Effect of Sb Segregation on Conductance and Catalytic Activity at Pt/Sb-Doped SnO\textsubscript{2} Interface: A Synergetic Computational and Experimental Study

Antimony doped tin dioxide (ATO) is considered a promising support material for Pt-based fuel cell cathodes, displaying enhanced stability over carbon-based supports. In this work, the effect of Sb segregation on the conductance and catalytic activity at Pt/ATO interface was investigated through a combined computational and experimental study. It was found that Sb-dopant atoms prefer to segregate toward the ATO/Pt interface. The deposited Pt catalysts, interestingly, not only promote Sb segregation, but also suppress the occurrence of Sb\textsuperscript{3+} species, a charge carrier neutralizer at the interface. The conductivity of ATO was found to increase, to a magnitude close to that of activated carbon, with an increment of Sb concentration before reaching a saturation point around 10%, and then decrease, indicating that Sb enrichment at the ATO surface may not always favor an increment of the electric current. In addition, the calculation results show that the presence of Sb dopants in ATO has little effect on the catalytic activity of deposited three-layer Pt toward the oxygen reduction reaction, although subsequent alloying of Pt and Sb could lower the corresponding catalytic activity. These findings help to support future applications of ATO/Pt-based materials as possible cathodes for PEMFC applications with enhanced durability under practical applications.
Effect of stress on NiO reduction in solid oxide fuel cells: A new application of energy-resolved neutron imaging

Recently, two new phenomena linking stress field and reduction rates in anode-supported solid oxide fuel cells (SOFCs) have been demonstrated, so-called accelerated creep during reduction and reduction rate enhancement and nucleation due to stress (Frandsen et al., 2014). These complex phenomena are difficult to study and it is demonstrated here that energy-resolved neutron imaging is a feasible technique for combined mechanics-chemical composition studies of SOFC components, including commercially produced ones. Cermet anode supports, which prior to the measurements were reduced under varying conditions such as different temperatures, various times and different values of applied stress, have been measured. Thus, samples with different contents (and gradients) of Ni and NiO phases were investigated. The
first Bragg edge transmission neutron measurements applied for the studies of the reduction progress in these samples were performed at two neutron beamline facilities (ISIS in the UK, Helmholtz Zentrum Berlin in Germany). The obtained results demonstrate the possibility to image and distinguish NiO and Ni phases within SOFC anode supports by energy-resolved neutron imaging and the potential of the neutron imaging method for in situ studies of reduction processes.

**General information**

State: Published
Organisations: Department of Energy Conversion and Storage, Rutherford Appleton Laboratory, European Spallation Source ESS AB, Helmholtz-Zentrum Berlin für Materialien und Energie, Xnovo Technology ApS, University of California at Berkeley
Authors: Makowska, M. (Intern), Strobl, M. (Ekstern), Lauridsen, E. M. (Ekstern), Frandsen, H. L. (Intern), Tremsin, A. S. (Ekstern), Kardjilov, N. (Ekstern), Manke, I. (Ekstern), Kelleher, J. F. (Ekstern), Kuhn, L. T. (Intern)
Number of pages: 8
Pages: 401-408
Publication date: 2015
Main Research Area: Technical/natural sciences

**Publication information**

Journal: Journal of Applied Crystallography
Volume: 48
ISSN (Print): 0021-8898
Ratings:
- BFI (2018): BFI-level 2
- BFI (2017): BFI-level 1
- Web of Science (2017): Indexed yes
- BFI (2016): BFI-level 1
- Scopus rating (2016): CiteScore 2.51 SJR 1.221 SNIP 1.211
- Web of Science (2016): Indexed yes
- BFI (2015): BFI-level 1
- Scopus rating (2015): SJR 2.271 SNIP 2.514 CiteScore 3.97
- Web of Science (2015): Indexed yes
- BFI (2014): BFI-level 1
- Scopus rating (2014): SJR 2.564 SNIP 4.297 CiteScore 4.76
- Web of Science (2014): Indexed yes
- BFI (2013): BFI-level 2
- Scopus rating (2013): SJR 2.934 SNIP 6.334 CiteScore 6
- ISI indexed (2013): ISI indexed yes
- Web of Science (2013): Indexed yes
- BFI (2012): BFI-level 2
- Scopus rating (2012): SJR 2.58 SNIP 4.659 CiteScore 4.67
- ISI indexed (2012): ISI indexed yes
- Web of Science (2012): Indexed yes
- BFI (2011): BFI-level 2
- Scopus rating (2011): SJR 3.818 SNIP 3.874 CiteScore 5.32
- ISI indexed (2011): ISI indexed yes
- Web of Science (2011): Indexed yes
- BFI (2010): BFI-level 2
- Scopus rating (2010): SJR 2.626 SNIP 2.056
- Web of Science (2010): Indexed yes
- BFI (2009): BFI-level 2
- Scopus rating (2009): SJR 3.265 SNIP 2.108
- Web of Science (2009): Indexed yes
- BFI (2008): BFI-level 2
- Scopus rating (2008): SJR 2.005 SNIP 2.545
- Web of Science (2008): Indexed yes
Effect of surface shear on cube texture formation in heavy cold-rolled Cu-45 at%Ni alloy substrates

Two types of Cu-45 at%Ni alloy thin tapes with and without surface shear were obtained by different heavy cold rolling processes. The deformation and recrystallization textures of the two tapes were thoroughly investigated by electron back scattering diffraction technique. The results showed that a shear texture mainly covered the surface of the heavy deformed tapes because of the fraction between the surface of rolling mills and the thin tapes when the rolling force strongly reduced at high strain, which significantly reduced the fraction of rolling texture on the surface of the Cu-45at %Ni alloy thin tapes, retarded the cube grain growth during recrystallization and affected the strong cube texture formation after high temperature annealing.

General information
State: Published
Organisations: Electrofunctional materials, Department of Energy Conversion and Storage, Beijing University of Technology
Authors: Tian, H. (Intern), Suo, H. (Ekstern), Liang, Y. (Ekstern), Yue, Z. (Intern), Grivel, J. (Intern)
Number of pages: 5
Pages: 83-87
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Materials Letters
Volume: 141
ISSN (Print): 0167-577X
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SJR 0.782 SNIP 0.887 CiteScore 2.68
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.51 SJR 0.754 SNIP 0.939
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Effect of Temperature Step Size on Calculating the Magnetic Entropy Change
Effects of constant voltage and constant current stress in PCBM:P3HT solar cells

The aim of this work is the investigation of forward and reverse bias stress effects, cell self-heating and annealing in roll coated organic solar cells with PCBM:P3HT active layer. In reverse bias stress cells show a constant degradation over time. In forward current stress cells alternate degradation and annealing phases, which are explained through the high power dissipation during the current stress, and the consequent self-heating. The high temperature is able to recover the cell performances at least until a critical temperature is reached. The degradation can be explained by the following mechanisms: the decrease of the net generation rate (due to formation of exciton quenching centres or the reduction of exciton separation rate); the formation of small leaky paths between anode and cathode, which reduces the total current extracted from the cell. The stress-induced damage can be recovered by thermal annealing at 120 °C. © 2015 Elsevier Ltd. All rights reserved.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Functional organic materials, University of Padova
Authors: Cester, A. (Ekstern), Rizzo, A. (Ekstern), Bazzega, A. (Ekstern), Lago, N. (Ekstern), Favaro, J. (Ekstern), Barbato, M. (Ekstern), Wrachien, N. (Ekstern), Gevorgyan, S. A. (Intern), Corazza, M. (Intern), Krebs, F. C. (Intern)
Number of pages: 5
Pages: 1795-1799
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication Information
Journal: Microelectronics Reliability
Volume: 55
ISSN (Print): 0026-2714
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 0.907 SJR 0.388 CiteScore 1.52
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.57 SJR 0.447 SNIP 0.991
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.581 SNIP 1.136 CiteScore 1.81
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.572 SNIP 1.376 CiteScore 1.9
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.568 SNIP 1.195 CiteScore 1.55
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.574 SNIP 1.323 CiteScore 1.6
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.607 SNIP 1.327 CiteScore 1.63
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.576 SNIP 1.064
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.686 SNIP 1.127
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 0.887 SNIP 1.228
Scopus rating (2007): SJR 0.733 SNIP 1.205
Effects of the fabrication process on the grain-boundary resistance in $\text{BaZr}_{0.9}\text{Y}_{0.1}\text{O}_{3-\delta}$

Correction for "Effects of the fabrication process on the grain-boundary resistance in $\text{BaZr0.9Y0.1O}_{3-\delta}$" by S. Ricote et al., J. Mater. Chem. A, 2014, 2, 16107–16115.
Effects of Yttrium and Iron co-doping on the high temperature thermoelectric properties of Ca$_3$Co$_4$O$_9$+$\delta$

A series of Y and Fe co-doped Ca$_{3-x}$Y$_x$Co$_{4-y}$FeyO$_9$+$\delta$ (0 $\leq$ x $\leq$ 0.3, 0 $\leq$ y $\leq$ 0.1) samples synthesized by auto-combustion reaction and followed by a spark plasma sintering (SPS) processing with the effects of Fe and Y doping on the high temperature (RT to 800 °C) thermoelectric properties were systematically investigated. For the Fe-doped system (x = 0, y = 0.1), the electrical resistivity ($\rho$) decreased over the whole measured temperature range, while the Seebeck coefficient ($S$) remained almost the same. For the co-doped system, at any fixed Fe doping content, both $\rho$ and $S$ tended to increase with increasing Y dopants, however, the effect is more substantial on $\rho$ than on $S$, particularly in the low temperature regime. In contrast to $\rho$ and $S$, the in-plane thermal conductivity ($\kappa$) is only slightly influenced by Y and Fe substitutions. Among all the investigated samples, the co-doped sample with x = 0.1 and y = 0.03 showed a decrease of $\rho$, enhanced power factor over the measured temperature range, and improved ZT at 800 °C as compared to un-doped Ca$_3$Co$_4$O$_9$+$\delta$. 

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials
Authors: Wu, N. (Intern), Van Nong, N. (Intern), Pryds, N. (Intern), Linderoth, S. (Intern)
Pages: 127–132
Publication date: 2015
Main Research Area: Technical/natural sciences
Elastocaloric cooling device: Materials and modeling

In the last decade we have witnessed the development of alternative solid-state cooling technologies based on so-called ferroic (caloric) effects. A large effort nowadays is devoted to investigating solid-state refrigeration using the magnetocaloric effect (change of temperature upon application of a magnetic field). However, the possibility of inducing a thermodynamic transition by means of mechanical stress (martensitic transformation), i.e. the elastocaloric effect in superelastic materials, opens up new routes for solid-state refrigeration. In the recent years a large elastocaloric effect was demonstrated in Ni-Ti-based, Cu-based as well as Fe-based shape memory alloys. Although these studies showed a great potential of the elastocaloric effect, there has not yet been much activities on development of elastocaloric cooling devices. Some ideas on elastocaloric cooling device have already been presented, but there is still a lack of knowledge and information about its actual cooling potential.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Department of Wind Energy, Composites and Materials Mechanics
Authors: Tusek, J. (Intern), Engelbrecht, K. (Intern), Pryds, N. (Intern), Mikkelsen, L. P. (Intern)
Number of pages: 2
Pages: 145-146
Publication date: 2015

Host publication information
Title of host publication: SMST 2015: The Model for Shape Memory Application, Proceedings of the Shape Memory and Superelastic Technologies Conference
Publisher: ASM International
Main Research Area: Technical/natural sciences
Conference: Shape Memory and Superelastic Technologies (SMST) Conference, Chipping Norton, Oxfordshire, United Kingdom, 18/05/2015 - 18/05/2015

DOI: 10.1016/j.jallcom.2015.02.185
Source: PublicationPreSubmission
Source-ID: 107843889
Publication: Research - peer-review › Journal article – Annual report year: 2015
Elastocaloric effect of Ni-Ti wire for application in a cooling device

We report on the elastocaloric effect of a superelastic Ni-Ti wire to be used in a cooling device. Initially, each evaluated wire was subjected to 400 loading/unloading training cycles in order to stabilize its superelastic behavior. The wires were trained at different temperatures, which lead to different stabilized superelastic behaviors. The stabilized (trained) wires were further tested isothermally (at low strain-rate) and adiabatically (at high strain-rate) at different temperatures (from 312 K to 342 K). We studied the impact of the training temperature and resulting superelastic behavior on the adiabatic temperature changes. The largest measured adiabatic temperature change during loading was 25 K with a corresponding 21K change during unloading (at 322 K). A special focus was put on the irreversibilities in the adiabatic temperature changes between loading and unloading. It was shown that there are two sources of the temperature irreversibilities: the hysteresis (and related entropy generation) and the temporary residual strain immediately after unloading, respectively. The latter results in the temporary bending of the wire and reduced negative adiabatic temperature change. The paper also shows the impact of the applied strain on the adiabatic temperature changes as well as the distribution of the elastocaloric effect over the wire during loading in the case of two wires trained at different temperatures and the virgin wire, respectively. In the end, we propose guidelines about the required material properties for an efficient elastocaloric cooling device. © 2015 AIP Publishing LLC.
Electrical characterization of fluorinated benzothiadiazole based conjugated copolymer – a promising material for high-performance solar cells

Measurements of electrical conductivity, electron work function, carrier mobility of holes and the diffusion length of excitons were performed on samples of conjugated polymers relevant to polymer solar cells. A state of the art fluorinated benzothiadiazole based conjugated copolymer (PBDTTTHD – DTBTff) was studied and benchmarked against the reference polymer poly-3-hexylthiophene (P3HT). We employed, respectively, four electrode conductivity measurements, Kelvin probe work function measurements, carrier mobility using charge extraction by linearly increasing voltage (CELIV) measurements and diffusion length determination using surface photovoltage measurements.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Functional organic materials, Charles University, Academy of Sciences of the Czech Republic
Authors: Toušek, J. (Ekstern), Toušková, J. (Ekstern), Remeš, Z. (Ekstern), Chomutová, R. (Ekstern), Čermák, J. (Ekstern), Helgesen, M. (Intern), Carlé, J. E. (Intern), Krebs, F. C. (Intern)
Number of pages: 8
Publication date: 2015
Main Research Area: Technical/natural sciences
Electrical properties and flux performance of composite ceramic hydrogen separation membranes

The electrical properties and hydrogen permeation flux behavior of the all-ceramic protonic/electronic conductor composite BaCe$_0.2$Zr$_{0.7}$Y$_{0.1}$O$_{3-\delta}$/Sr$_{0.95}$Ti$_{0.9}$Nb$_{0.1}$O$_{3-\delta}$ (BCZY27/STN95: BS27) are evaluated. Conductivity and hydrogen permeability are examined as a function of phase volume ratios. Total conductivities of 0.01-0.06 S cm$^{-1}$ are obtained in moist (+1% H$_2$O) H$_2$/inert gas from 600-800 °C for 50 volume% STN95. With increasing STN95 content (60 and 70 volume%), conductivity increases by 5-10 times, but displays a semiconductor-type dependence, even at 70 volume% STN95. The conductivity is modeled with an effective medium approach incorporating a term for the heterojunctions between the two phases. Hydrogen fluxes of 0.004-0.008 μmol cm$^{-2}$ s$^{-1}$ are obtained for a 50 volume% STN95 membrane sample (1 mm thickness) at 600-800 °C using dry argon as a sweep gas. Upon adding palladium layers as catalysts more than a five-fold increase is observed in the hydrogen flux, 0.025-0.026 μmol cm$^{-2}$ s$^{-1}$, over the same temperature range. Hydrogen flux is not observed for membranes made from the 60 and 70% STN95 samples.
The electrochemical reduction of NO with propene in the presence of oxygen on LSCoM/CGO porous cell stacks impregnated with BaO was studied on a La0.85Sr0.15Co0.03Mn0.97O3-Ce0.9Gd0.1O1.95 11-layer electrochemical reactor. BaO was impregnated into the porous reactor, and electrochemical impedance spectroscopy was used for characterisation in the temperature range of 300–400 °C. They were subjected to different magnitudes of polarisations, and the BaO impregnation was shown to have increased the NO reduction with increasing polarisation in the presence of excess oxygen. At 350 °C, more than 60 % was removed and a current efficiency for the cell stack of up to 30 % was achieved. In the presence of propene, the electrochemical promotion on the NOx conversion decreased and only 13 % was removed. A propene oxidation of 35 % was achieved as the highest at 400 °C. The propene acted as a reducing agent on the barium nitrates and caused a greater reduction of the nitrates and hereby releasing more NO than in the gas without propene. This caused an increase in NO in the outlet gas since not all of it was reduced further to nitrogen. The results indicate that the electrochemical
reduction of the nitrates when no propene is present is a surface reaction, whereas the propene enables further reduction of the bulk nitrate.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Fundamental Electrochemistry
Authors: Friedberg, A. Z. (Intern), Kammer Hansen, K. (Intern)
Number of pages: 10
Pages: 1611-1620
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Solid State Electrochemistry
Volume: 19
Issue number: 6
ISSN (Print): 1432-8488
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 0.674 SJR 0.661 CiteScore 2.37
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.26 SJR 0.678 SNIP 0.735
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.643 SNIP 0.68 CiteScore 2.18
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.831 SNIP 0.996 CiteScore 2.59
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.734 SNIP 0.918 CiteScore 2.25
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.875 SNIP 1 CiteScore 2.23
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.868 SNIP 0.994 CiteScore 2.28
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.897 SNIP 0.97
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.849 SNIP 0.907
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.755 SNIP 0.725
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.778 SNIP 0.773
Scopus rating (2006): SJR 0.784 SNIP 0.976
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.634 SNIP 0.839
Electrochemistry as a Tool for Study, Development and Promotion of Catalytic Reactions

The first two chapters of the dissertation are dedicated to definition of the peculiarities of electrochemical processes and also common features and differences between heterogeneous redox and catalytic reactions and electrochemical reactions. The main common characteristic of heterogeneous catalytic reactions and electrochemical reactions is defined. It is the Fermi level of the catalyst, which is also the electrochemical potential of the electrode. According to the Newns-Anderson theory, Fermi level of catalysts affects (or even define) their activity. The electrochemical potential can be measured and changed by polarization in electrochemical experiment. In Chapter 3 the nature of the electrochemical heterogeneous catalytic reactions is discussed, including the new theory of electrochemical promotion. This theory is based on electrochemical change of the Fermi level of the catalyst. It also states that that there are two types of electrochemical promotion: First type is based on change of the Fermi level through the charge of the electric double layer (EDL) between catalyst and its support without electrochemical reaction. This effect was abbreviated as EDLE. Second type is based on change of Fermi level by electrochemical production of promoters, reducing or oxidizing current carriers of the catalyst support (O2-, H+, Na+). This type was abbreviated as EEPP. In Chapters 4-7, the results of my research are given as examples of use of electrochemistry as a tool for study, promotion and development of catalysts.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors
Authors: Petrushina, I. (Intern)
Number of pages: 187
Publication date: 2015

Publication information
Place of publication: Kgs. Lyngby
Publisher: Department of Energy Conversion and Storage, Technical University of Denmark
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
Electrochemistry_as_a_Tool_for_Study.pdf

Bibliographical note
The defence will take place on Monday, 2 November 2015
Publication: Research › Doctoral thesis – Annual report year: 2015
diffusion through the porous electrodes, activation or charge transfer at the reaction sites, gas conversion at the reaction sites and flow fields and ohmic drop across the electrolyte. These processes occur in both electrodes and often their characteristic frequencies overlap, rendering characterization of a given mechanism particularly challenging. To optimize the SOCs for operation in the different fuels, operation temperature and operation modes it is important to understand the kinetics of the SOC electrodes. This thesis was aimed at understanding the kinetics of the SOC under different operation conditions of temperature, polarization, and fuel mixture. For investigations on full cells, electrochemical impedance spectroscopy and distribution of relaxation times techniques were used to investigate kinetics of the Ni/YSZ fuel electrode in three fuel mixtures – hydrogen/steam and reformate fuels hydrogen/carbon-dioxide and hydrogen/methane/steam. It was found that the kinetics at the fuel electrode were exactly the same in both reformates. This means that chemical equilibrium reactions were much faster than the electrochemical reactions. The electrode displayed slightly faster kinetics in hydrogen/steam fuel than in the reformate fuels.

To minimize the influence of (i) joule heating effects as a result of current flow across the electrolyte, (ii) concentration-related effects like gas diffusion, and (iii) overlapping of the characteristic frequencies of processes, the investigations were extended from full cell geometries to a novel pseudo-three electrode cell geometry with working-electrode areas of ca. 1 mm² that enabled isolated investigation of the fuel and oxygen electrodes. In a 50/50 H2/H2O fuel mixture, the Ni/8 mol % yttria-stabilized zirconia (Ni/YSZ) fuel electrode showed slower reaction kinetics operating under cathodic polarization than anodic—the same finding had been reported in literature from investigations on full cells whereby together with the local pH2O, substrate diffusion (specifically Knudsen diffusion) was identified as one of the causes of asymmetry between anodic and cathodic mode polarization. Obtained charge-transfer coefficients compared well with those reported in literature and their evolution with temperature was similar to that reported in literature based on porous Ni/YSZ fuel electrodes. From the two investigated oxygen electrodes, the higher performing (La0.58Sr0.4)0.99CoO3/Co0.99d0.101.95 (LSC/CGO) oxygen electrode showed slower reaction kinetics under cathodic mode operation at 50 mV overvoltage than in anodic mode. The trend was opposite for the lower performing La0.58Sr0.4Co0.2Fe0.8O3 (LSCF) oxygen electrode. However, with decreasing oxygen partial pressure both electrodes displayed increasing asymmetry between anodic and cathodic modes. It could be shown that surface exchange kinetics were the major cause of the decreasing kinetics with decreasing pO2 and that the cathodic mode kinetics were slowed down much more than the anodic branch kinetics thus increasing the asymmetry.

Independent of operation mode, commercialization of the SOC technology requires a guarantee of longevity as well as predictability of the SOC performance under desired operation conditions.

The performance is generally evaluated through the current/voltage (C/V) curve. As such, a deviation from the expected/predicted performance curve can serve to identify the presence of ageing or an ageing inducing process. A 0-D stationary model was previously developed at the Institut für Angewandte Materialien - Werkstoffe der Elektrotechnik (IAM-WET) in Germany to predict the C/V curve of a SOC for fuel cell operation mode. In this thesis, the applicability of this model was verified for electrolysis mode operation, the model was extended to accommodate temperature changes under polarization in fuel cell and electrolysis mode operation, and the model was further extended to cover operation in reformate fuels H2/H2O/CO/CO2. The latter was accomplished by including a new concentration-related overpotential contribution in the model to account for the CO/CO2 diffusion to the reaction sites as a result of the water gas shift equilibrium reactions.

The long-term stability of the system depends on whether the system is operated solely in fuel-, electrolysis-, reversible or dynamic mode. Optimization of the cells for high performance and/or durability in each of these operation modes requires a thorough understanding of the processes and mechanisms affecting the kinetics and ageing of the systems. In five tests with varying durations between 1000 h and 2500 h the long-term stability of the SOCs was investigated for constant electrolysis, cyclic and dynamic operation modes in a symmetric binary fuel of 50/50 H2/H2O at 800 °C and 700 °C. The SOCs investigated under constant electrolysis mode aged more than those investigated under cyclic mode with the fuel electrode dominating the ageing in constant electrolysis mode and the oxygen electrode dominating that in cyclic mode. During dynamic cycling, the SOCs aged less at 800 °C than at 700 °C. It was observed that for cycles with equal durations in SOEC and SOFC modes whereby the cycle lengths were less than or equal to 2 x 5 h the voltage ageing was almost symmetrical for both SOFC and SOEC modes. For longer cycle lengths SOEC mode voltage ageing was at least double the SOFC mode voltage ageing. This result is consistent with suggestions in literature that intermittent operation of SOCs in fuel cell mode slows down or even reverses SOC ageing that occurs during long-term electrolysis operation. Based on the findings that the fuel electrode dominated the ageing under constant electrolysis operation, it was speculated that surface exchange kinetics, to be caused by precipitation of nickel oxide that had diffused into the 8YSZ matrix of the fuel electrode during sintering.

Constant electrolysis operation provided enhanced conditions for the precipitation of the nickel oxide as metallic nickel. Furthermore, Zr, Ni, Y, and O containing nano-particles were found on the Ni particles. In literature during electrolysis of H2/O2 under same conditions of temperature and current density nano particles were also found on Ni particles, identified as ZrO2 and attributed the major cause of fuel electrode ageing. In cyclic operation these enhancing conditions were not maintained long-enough for severe nickel precipitation. It is known and was verified that the LSC/CGO electrode is better performing than the LSCF electrode. To compare the stability of these two state-of-the-art (s.t.a.) oxygen electrodes, 1000 h tests under non-polarized or open circuit voltage (OCV) conditions were carried out using symmetric cell geometry. Both electrodes displayed a two-step ageing trend with rapid initial ageing within the first 400 h followed by relaxation to slower ageing rates. The LSCF electrode showed a larger increase in polarization resistance especially within the first 400 h in which it aged by factor 6 faster than the LSC/CGO electrode. The rapid ageing of the LSCF electrode within the first 300 – 400 h of operation has also been reported in literature.
Electrophoretic deposition of Mn$_{1.5}$Co$_{1.5}$O$_4$ on metallic interconnect and interaction with glass-ceramic sealant for solid oxide fuel cells application

Cr-containing stainless steels are widely used as metallic interconnects for SOFCs. Volatile Cr-containing species, which originate from the oxide formed on steel, can poison the cathode material and subsequently cause degradation in the SOFC stack. Mn$_{1.5}$Co$_{1.5}$O$_4$ spinel is one of the most promising coating materials due to its high electrical conductivity, good CTE match with the stainless steel substrate and an excellent chromium retention capability. In this work Mn$_{1.5}$Co$_{1.5}$O$_4$ spinel coatings are deposited on Crofer22APU substrates by cathodic electrophoretic deposition (EPD) followed by sintering at 800-1150 °C in different atmospheres. Dense, continuous and crack free Mn$_{1.5}$Co$_{1.5}$O$_4$ coatings (with thickness ranging from 10 to 40 μm) are obtained on Crofer22APU substrates. Moreover, electrical properties of the coated Crofer22APU alloy are tested up to 2500 h and an excellent compatibility is found between Mn$_{1.5}$Co$_{1.5}$O$_4$ coated Crofer22APU and a new glass-ceramic sealant, after 500 h of thermal tests in air, thus suggesting that the spinel protection layer can effectively act as a barrier to outward diffusion of Cr. [All rights reserved Elsevier].

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Politecnico di Torino, University of Erlangen-Nuremberg
Authors: Smeacetto, F. (Ekstern), De Miranda, A. (Ekstern), Cabanas Polo, S. (Ekstern), Molin, S. (Intern), Boccaccini, D. (Intern), Salvo, M. (Ekstern), Boccaccini, A. R. (Ekstern)
Number of pages: 8
Pages: 379-386
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Power Sources
Volume: 280
Electrospinning for Solid Oxide Fuel Cells

General information
State: Published
Organizations: Department of Energy Conversion and Storage, Ceramic Engineering & Science
Authors: Zhang, W. (. (Intern)
Pages: 61-76
Publication date: 2015

Host publication information
Title of host publication: Electrospinning for Advanced Energy and Environmental Applications
Publisher: CRC Press, Taylor & Francis Group
Editor: Cavaliere, S.
ISBN (Print): 978-1-4822-1767-4
ISBN (Electronic): 978-1-4822-1768-1
Chapter: 3
Main Research Area: Technical/natural sciences
Source: PublicationPreSubmission
Source-ID: 129007481
Publication date: 2015

Eliminating degradation in solid oxide electrochemical cells by reversible operation

General information
State: Published
Organizations: Department of Energy Conversion and Storage, Applied Electrochemistry, Imaging and Structural Analysis, Fundamental Electrochemistry
Authors: Graves, C. R. (Intern), Ebbesen, S. D. (Intern), Jensen, S. H. (Intern), Simonsen, S. B. (Intern), Mogensen, M. B. (Intern)
Number of pages: 6
Pages: 239–244
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Nature Materials
Volume: 14
ISSN (Print): 1476-1122
Ratings:
BFI (2018): BFI-level 3
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): SJR 18.263 SNIP 8.977 CiteScore 25.47
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 23.67 SJR 18.013 SNIP 9.04
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 14.956 SNIP 8.905 CiteScore 23.23
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 16.726 SNIP 9.171 CiteScore 23.3
ISI indexed (2013): ISI indexed yes
Enabling Flexible Polymer Tandem Solar Cells by 3D Ptychographic Imaging

The realization of a complete tandem polymer solar cell under ambient conditions using only printing and coating methods on a flexible substrate results in a fully scalable process but also requires accurate control during layer formation to succeed. The serial process where the layers are added one after the other by wet processing leaves plenty of room for error and the process development calls for an analytical technique that enables 3D reconstruction of the layer stack with the possibility to probe thickness, density, and chemistry of the individual layers in the stack. The use of ptychography on a complete 12-layer solar cell stack is presented and it is shown that this technique provides the necessary insight to enable efficient development of inks and processes for the most critical layers in the tandem stack such as the recombination layer where solvent penetration in fully solution processed 12-layer stacks is critical in eleven of the steps.

General information

State: Published
Organisations: Department of Energy Conversion and Storage, Functional organic materials, Imaging and Structural Analysis, Deutsches Elektronen-Synchrotron
Number of pages: 6
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information

Journal: Advanced Energy Materials
Volume: 5
Issue number: 1
Article number: 1400736
ISSN (Print): 1614-6832
In this article we discuss the synthesis of four new low band-gap co-polymers based on the diketopyrrolopyrrole (DPP) and benzotriazole (BTZ) monomer unit. We demonstrate that the BTZ unit allows for additional solubilizing side-chains on the co-monomer and show that the introduction of a linear side-chain on the DPP-unit leads to an increase in thin-film order and charge-carrier mobility if a sufficiently solubilizing, branched, side chain is attached to the BTZ. We compare two different synthetic routes, direct arylation and Suzuki-polycondensation, by a direct comparison of polymers obtained via the two routes and show that direct arylation produces polymers with lower electrical performance which we attribute to a higher density of chain. Furthermore we demonstrate that a polymer utilizing this design motif and synthesized via Suzuki-polycondensation ((l-C18)-DPP-(b-C17)-BTZ) exhibits exceptionally high and near balanced average electron and hole mobilities >2 cm² V⁻¹ s⁻¹ which are among the highest, robustly extracted mobility values reported for DPP copolymers in a top-gate configuration to date. Our results demonstrate clearly that linear side chain substitution of the DPP unit together with co-monomers that allow for the use of sufficiently long or branched solubilizing side chains can be an attractive design motif for solution processable, high mobility DPP copolymers.
Energy Supply Modelling in Cities, Illustrated Using Data from the Municipality of Sønderborg in Denmark

In the ongoing transition towards a fully sustainable energy system, maximizing the system efficiency and the integration across its sectors while minimizing the costs of the system and carefully prioritizing the usage of energy resources are key issues. Denmark aims at becoming independent of fossil fuels for electricity and heat generation by 2035 and at having a fully renewable energy system by 2050. Harmonized national and regional efforts are required in order to meet these goals. As the majority of the demand for energy services is located in cities, it is useful to focus on city areas when seeking to optimize the system efficiency, economy and integration. We have performed a case study using data from the Danish municipality of Sønderborg, which has the goal of becoming CO2 neutral by 2029. We have developed and modeled different scenarios for Sønderborg’s energy system in 2029, containing various different energy conversion pathways. These include e.g. biogas production and upgrade using hydrogen from electrolysis, scenarios with biomass gasification and local transport fuel production and scenarios in which gas turbines for reserve electricity generation have been displaced by reversible electrolysis/fuel cell systems. The aim of the case study was to identify if and how new energy conversion technologies can be integrated in the future energy system to meet the demand for energy services in an economical, efficient and sustainable way on a regional scale. The results show that the gas and district-heating systems, along with utility-scale heat pumps, will serve as valuable system integrators for the large amounts of fluctuating electricity supply from wind and PV. The overall system efficiency can be enhanced by supplying surplus process heat to the district-heating network and by using electrolysis to produce hydrogen for upgrading of biomass-derived gases. The results also pinpoint the importance of prioritizing biomass for the production of synthetic hydrocarbon transport fuels rather than for heat and power generation. The work was carried out using the Sifre energy systems analysis software developed by Energinet.dk
(the Danish electricity and gas TSO). It is a linear optimization model that seeks a least-cost solution for the hour-by-hour operation of the specified energy system. The work was carried out as part of CITIES, funded by Innovation Fund Denmark.

**General information**

**State:** Published  
**Organisations:** Department of Energy Conversion and Storage, Centre for IT-Intelligent Energy Systems in Cities, Energinet.dk  
**Authors:** Sveinbjörnsson, D. Þ. (Intern), Algren, L. (Ekstern), Bavnhøj Hansen, A. (Ekstern), Pedersen, A. S. (Intern)  
**Publication date:** 2015  
**Event:** Abstract from 10th Conference on Sustainable Development of Energy, Water and Environment Systems, Dubrovnik, Croatia.  
**Main Research Area:** Technical/natural sciences  
**Source:** PublicationPreSubmission  
**Source-ID:** 117919875  
**Publication:** Research - peer-review › Conference abstract for conference – Annual report year: 2015

**Enhanced reducibility and electronic conductivity of Nb or W doped Ce$_{0.9}$Gd$_{0.1}$O$_{1.95-\delta}$**

The transport and thermomechanical properties of acceptor (Gd) and donor (Nb or W) co-doped ceria were investigated. The solubility limit of Nb in Ce$_{0.9}$Gd$_{0.1}$O$_{2-\delta}$ (CGO10) exceeds 4 at.%, whereas that of W is approximately 2 at.%. Both the thermal and stoichiometric expansion coefficients are decreased relative to that of CGO10. Charge compensation of the donor dopants takes place primarily by annihilation of oxide ion vacancies, and a sharp decrease in ionic mobility is observed upon Nb or W doping of CGO10. On the other hand, the n-type electronic conductivity, associated with the reduction of Ce$^{4+}$, increases upon doping with Nb or W, due to enhanced reducibility of cerium. This is beneficial for applications where electronic conductivity is also required, like oxygen permeation membranes. Modeling shows that 4 at.% Nb or W doped CGO10 will deliver higher oxygen fluxes than CGO10, due to the enhanced electronic conductivity and despite the reduced ionic conductivity.

**General information**

**State:** Published  
**Organisations:** Department of Energy Conversion and Storage, Fundamental Electrochemistry, Ceramic Engineering & Science, Mixed Conductors  
**Authors:** Chatzichristodoulou, C. (Intern), Ricote, S. (Intern), Foghmoes, S. P. V. (Intern), Glasscock, J. (Intern), Kaiser, A. (Intern), Hendriksen, P. V. (Intern)  
**Number of pages:** 6  
**Pages:** 51-56  
**Publication date:** 2015  
**Main Research Area:** Technical/natural sciences

**Publication information**

**Journal:** Solid State Ionics  
**Volume:** 269  
**ISSN (Print):** 0167-2738  
**Ratings:**  
  - BFI (2018): BFI-level 1  
  - Web of Science (2018): Indexed yes  
  - BFI (2017): BFI-level 1  
  - Scopus rating (2017): CiteScore 2.64 SJR 0.856 SNIP 0.952  
  - Web of Science (2017): Indexed yes  
  - BFI (2016): BFI-level 1  
  - Scopus rating (2016): CiteScore 2.41 SJR 0.75 SNIP 0.909  
  - Web of Science (2016): Indexed yes  
  - BFI (2015): BFI-level 1  
  - Scopus rating (2015): SJR 0.802 SNIP 1.016 CiteScore 2.5  
  - Web of Science (2015): Indexed yes  
  - BFI (2014): BFI-level 1  
  - Scopus rating (2014): SJR 0.837 SNIP 1.282 CiteScore 2.62  
  - Web of Science (2014): Indexed yes  
  - BFI (2013): BFI-level 1  
  - Scopus rating (2013): SJR 0.903 SNIP 1.269 CiteScore 2.35  
  - ISI indexed (2013): ISI indexed yes
Enhancement of the chemical stability in confined δ-Bi₂O₃

Bismuth-oxide-based materials are the building blocks for modern ferroelectrics, multiferroics, gas sensors, light photocatalysts and fuel cells. Although the cubic fluorite δ-phase of bismuth oxide (δ-Bi₂O₃) exhibits the highest conductivity of known solid-state oxygen ion conductors, its instability prevents use at low temperature. Here we demonstrate the possibility of stabilizing δ-Bi₂O₃ using highly coherent interfaces of alternating layers of Er₂O₃-stabilized δ-Bi₂O₃ and Gd₂O₃-doped CeO₂. Remarkably, an exceptionally high chemical stability in reducing conditions and redox cycles at high temperature is achieved. Even more interestingly, at low oxygen partial pressure the layered material shows anomalous high conductivity, equal or superior to pure δ-Bi₂O₃ in air. This suggests a strategy to design and stabilize new materials that are comprised of intrinsically unstable but high-performing component materials.
Enhancing hybrid direct carbon fuel cell anode performance using Ag$_2$O

A hybrid-direct carbon fuel cell (HDCFC), consisting of a molten slurry of solid carbon black and (Li-K)$_2$CO$_3$ added to the anode chamber of a solid oxide fuel cell, was characterized using current-potential-power density curves, electrochemical impedance spectroscopy, and cyclic voltammetry. Two types of experimental setups were employed in this study, an anode-supported full cell configuration (two electrodes, two atmospheres setup) and a 3-electrode electrolyte-supported half-cell setup (single atmosphere). Anode processes with and without catalysts were investigated as a function of temperature (700-800 °C) and anode sweep gas (N$_2$, 4-100% CO$_2$ in N$_2$-CO$_2$). It was shown that the addition of silver based catalysts (Ag, Ag$_2$O, Ag$_2$CO$_3$) into the carbon-carbonate slurry enhanced the performance of the HDCFC.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Fundamental Electrochemistry
Authors: Deleebeeck, L. (Intern), Ippolito, D. (Intern), Kammer Hansen, K. (Intern)
Number of pages: 18
Pages: 222-239
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Electrochimica Acta
Volume: 152
ISSN (Print): 0013-4686
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 5.01 SJR 1.439 SNIP 1.101
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.74 SJR 1.355 SNIP 1.177
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.321 SNIP 1.324 CiteScore 4.86
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.378 SNIP 1.456 CiteScore 4.59
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.427 SNIP 1.587 CiteScore 4.44
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.644 SNIP 1.574 CiteScore 3.99
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
Environmental benefits of parking-integrated photovoltaics: A 222kWp experience

The life cycle assessment of a grid-connected, parking integrated, 222kWp cadmium telluride photovoltaic system has been performed. The system was built at the University of Murcia and has been monitored for 2.5 years (sampling data every 5 min). The detailed material inventory, the energy embedded in the system, the energy payback time, and the energy return factor of the facility have been obtained and are 6.31TJ equivalent primary energy, 2.06 and 12.16 years, respectively. The average performance ratio is 0.8 with a slight monthly variation. Additionally, the environmental benefits of the architectural integration (in this case parking integration) have been quantified using a standard methodology for the calculation of several environmental parameters. Finally, the environmental benefits of renewable energy generation because of the savings of producing the same amount of electricity by the Spanish grid system have been assessed. © 2013 John Wiley & Sons, Ltd.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Functional organic materials, Imperial College London, Universidad Politecnica de Cartagena
Authors: Serrano-Luján, L. (Ekstern), García-Valverde, R. (Ekstern), Espinosa, N. (Intern), García-Cascales, M. S. (Ekstern), Sánchez-Lozano, J. M. (Ekstern), Urbina, A. (Ekstern)
Pages: 253-264
Publication date: 2015
Environmental impacts of electricity generation at global, regional and national scales in 1980–2011: What can we learn for future energy planning?

The generation of electricity has been known to cause important damages to ecosystems and human health. The recognition of the global challenges posed by climate change and energy security has guided several countries to change their electricity policies over the past decades. However, have such changes entailed reduced or increased environmental impacts? Are there any identifiable patterns that could serve for steering future energy planning? To address these questions, we applied life cycle assessment to quantify a whole spectrum of environmental impacts caused by electricity generation in 199 countries for the period 1980–2011, with national differentiation of energy sources and, wherever possible, technology efficiencies. The results show that (i) environmental impact burden-shifting has occurred in the past for several countries as a result of national policies, (ii) all environmental impacts have globally increased since 1980 but with faster increase rates over the last decade, and (iii) important variations exist in the impact trends across countries and across impact categories. Our findings therefore demonstrate the need for integrating quantitative assessments of all relevant environmental impacts associated with foreseen energy systems when identifying the most sustainable energy pathways. We provide recommendations on the use of life cycle assessment for such purposes with a strong focus on application at the country level so that it can directly support national energy policy-making.

General information
State: Published
Organisations: Department of Management Engineering, Quantitative Sustainability Assessment, Department of Energy Conversion and Storage, Functional organic materials
Authors: Laurent, A. (Intern), Espinosa Martinez, N. (Intern)
Pages: 689–701
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Energy & Environmental Science
Volume: 8
ISSN (Print): 1754-5692
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): SNIP 4.819 SJR 14.59 CiteScore 30.87
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 26.39 SJR 12.283 SNIP 4.325
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 7.769 SNIP 4.001 CiteScore 19.28
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 6.019 SNIP 2.996 CiteScore 14.81
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 5.868 SNIP 2.599 CiteScore 11.84
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 3.737 SNIP 2.505 CiteScore 9.96
ISI indexed (2011): ISI indexed no
Web of Science (2011): Indexed yes
Environmental TEM study of the dynamic nanoscaled morphology of NiO/YSZ during reduction

The reduction of a metal oxide is often a critical preparation step for activating catalytic behaviour. This study addresses the reduction process of NiO in pure form and in a composite of NiO/yttria-stabilized zirconia (YSZ) in hydrogen relevant for solid oxide electrochemical cells by comparing results from environmental transmission electron microscopy (ETEM) with thermogravimetric analysis (TGA). The temperature dependent reduction profiles obtained from TGA confirm an inhibitive effect from YSZ on the NiO reduction. The ETEM images show the growth of Ni in decaying NiO and reveal the nanoscale morphological changes such as pore formation in NiO above 280°C and densification and collapse of the pore structures above 400°C. The accelerated Ni front in NiO illustrates the auto catalysis of the reaction. A rapid temperature ramping from room temperature to 780°C in hydrogen in 1 second resulted in immediate morphological changes at the nanoscale from dense NiO to dense Ni. The analysis suggests that the inhibitive effect of YSZ on the NiO reduction reaction is not due to a direct local interaction between YSZ and NiO, but instead due to gas and/or mass transport limitations.© 2014 Elsevier B.V. All rights reserved.
Er der vedvarende energi nok til os alle?: om brændselsceller og elektrolyseceller til effektiv energikonvertering

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry
Authors: Hauch, A. (Intern)
Number of pages: 29
Publication date: 2015

Publication information
Media of output: PowerPoint
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
Br_nsdelsceller_og_elektrolyseceller_DanskNaturvidenskabsfestival_AnneHauch_September26th2014.pdf
**Experimental Studies with an Active Magnetic Regenerating Refrigerator**

Experimental results for an active magnetic regenerator (AMR) are presented. The focus is on whether or not it pays off to partly substitute soft magnetic material with non-magnetic insulation in a flux-conducting core in the magnet system. Such a substitution reduces losses due to heat conduction and eddy currents, but also reduces the magnetic field. Two different cores were tested in the AMR system with different cooling loads and it is shown, that in the present case, replacing half of the iron with insulation lead to an average reduction in temperature span of 14%, but also a small decrease in COP, hence the substitution did not pay off. Furthermore, it is shown experimentally, that small imbalances in the heat transfer fluid flow greatly influence the system performance. A reduction of these imbalances through valve adjustments resulted in an increase in the temperature span from approximately 16 K to 27.3 K.

**Extreme mobility enhancement of two-dimensional electron gases at oxide interfaces via charge transfer induced modulation doping**

The discovery of two-dimensional electron gases (2DEGs) at the interface between two insulating complex oxides, such as LaAlO3 (LAO) or gamma-Al2O3 (GAO) epitaxially grown on SrTiO3 (STO), provides an opportunity for developing all-oxide electronic devices. These 2DEGs at complex oxide interfaces involve many-body interactions and give rise to a rich set of phenomena, for example, superconductivity, magnetism, tunable metal-insulator transitions, and phase separation. However, large enhancement of the interfacial electron mobility remains a major and long-standing challenge for fundamental as well as applied research of complex oxides. Here, we inserted a single unit cell insulating layer of polar La1-xSrxF3O3 (x=0, 1/8, and 1/3) at the interface between disordered LaAlO3 and crystalline SrTiO3 created at room temperature. We find that the electron mobility of the interfacial 2DEG is enhanced by more than two orders of magnitude.
Our in-situ and resonant x-ray spectroscopic in addition to transmission electron microscopy results indicate that the manganite layer undergoes unambiguous electronic reconstruction and leads to modulation doping of such atomically engineered complex oxide heterointerfaces. At low temperatures, the modulation-doped 2DEG exhibits clear Shubnikov-de Haas oscillations and the initial manifestation of the quantum Hall effect, demonstrating an unprecedented high-mobility and low electron density oxide 2DEG system. These findings open new avenues for oxide electronics.
Extreme mobility enhancement of two-dimensional electron gases at oxide interfaces via charge transfer induced modulation doping

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, University of Twente, University of British Columbia, University of Antwerp, University of Saskatchewan, Weizmann Institute of Science, University of Copenhagen
Number of pages: 2
Publication date: 2015
Event: Abstract from 22nd International Workshop on Oxide Electronics, Paris, France.
Main Research Area: Technical/natural sciences
Electronic versions:
Extreme_mobility Enhancement.pdf
Publication: Research - peer-review › Journal article – Annual report year: 2015

Extreme mobility enhancement of two-dimensional electron gases at oxide interfaces via charge transfer induced modulation doping

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, University of Twente, University of British Columbia, University of Antwerp, University of Saskatchewan, Weizmann Institute of Science, University of Copenhagen
Number of pages: 1
Publication date: 2015
Event: Poster session presented at E-MRS 2015 Fall meeting, Warsaw, Poland.
Main Research Area: Technical/natural sciences
Electronic versions:
Extreme_mobility Enhancement_poster.pdf
Fabrication and performance of a tubular ceria based oxygen transport membrane on a low cost MgO support

A 30 μm thin-film tubular CGO (Ce$_{0.9}$Gd$_{0.1}$O$_{1.95-δ}$) membrane with catalytic layers on both sides has been prepared by dip-coating on a low cost, porous magnesium oxide (MgO) support. The MgO support was fabricated through a thermoplastic extrusion process. Support, thin membrane and catalytic layers were sintered in individual steps at temperatures between 1250 and 1300 °C to achieve a controlled removal of binder and organic additives and to obtain the desired, defect free microstructure. The prepared asymmetric tubular CGO membrane has been tested at elevated temperatures (up to 900 °C) using atmospheric air and N$_2$, H$_2$ for the feed and sweep side respectively. The oxygen permeation was 4 N ml min$^{-1}$ cm$^{-2}$ at 850 °C using H$_2$ on one side and air on the other side.

**General information**
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Mixed Conductors, Swiss Federal Laboratories for Materials Testing and Research
Authors: Kothanda Ramachandran, D. (Intern), Søgaard, M. (Intern), Clemens, F. (Ekstern), Gurauskis, J. (Intern), Kaiser, A. (Intern)
Pages: 422–430
Publication date: 2015
Main Research Area: Technical/natural sciences

**Publication information**
Journal: Separation and Purification Technology
Volume: 147
ISSN (Print): 1383-5866
Ratings:
- BFI (2018): BFI-level 2
- Web of Science (2018): Indexed yes
- BFI (2017): BFI-level 2
- Scopus rating (2017): SNIP 1.475 SJR 1.093 CiteScore 4.25
- Web of Science (2017): Indexed yes
- BFI (2016): BFI-level 2
- Scopus rating (2016): CiteScore 3.78 SJR 1.024 SNIP 1.4
- Web of Science (2016): Indexed yes
- BFI (2015): BFI-level 2
- Scopus rating (2015): SJR 1.07 SNIP 1.499 CiteScore 3.75
- Web of Science (2015): Indexed yes
- BFI (2014): BFI-level 2
- Scopus rating (2014): SJR 1.261 SNIP 1.532 CiteScore 3.5
- Web of Science (2014): Indexed yes
- BFI (2013): BFI-level 2
- Scopus rating (2013): SJR 1.327 SNIP 1.674 CiteScore 3.62
- ISI indexed (2013): ISI indexed yes
- Web of Science (2013): Indexed yes
- BFI (2012): BFI-level 2
- Scopus rating (2012): SJR 1.394 SNIP 1.718 CiteScore 3.2
- ISI indexed (2012): ISI indexed yes
- Web of Science (2012): Indexed yes
- BFI (2011): BFI-level 2
- Scopus rating (2011): SJR 1.352 SNIP 1.633 CiteScore 3.48
- ISI indexed (2011): ISI indexed yes
- Web of Science (2011): Indexed yes
- BFI (2010): BFI-level 2
- Scopus rating (2010): SJR 1.386 SNIP 1.58
- BFI (2009): BFI-level 2
- Scopus rating (2009): SJR 1.386 SNIP 1.536
- Web of Science (2009): Indexed yes
Fabrication of doped Titania (TiO2) nano-catalysts in the shape of nanofibers

Nanostructured materials have attracted incredible interest during the recent years for a large variety of applications. In heterogeneous catalysis the use of nano-sized catalytic materials is expected to significantly impact the performances of materials as consequence of their large surface-to-volume ratios [1]. The “nanomaterial” approach enables to achieve structures with incredible large exposed surface area. When nanofibers are used as nano-catalysts, the further advantage of a quite open porous structure is further achieved. In this work, nanomaterial approach was adopted to fabricate nano-catalysts for the removal of the NOx in exhausts via the NH3 Selective Catalytic Reduction method (SCR). The state-of-art system WO3-V2O5 was incorporated into TiO2 ceramic nanofibers through combination of electrospinning and sol-gel process. Catalytic functionalized nanofibers were characterized using SEM, TEM, EDX, BET, XRD, to analyze fiber diameter, morphology, composition, specific surface area, crystallization phases of TiO2 functionalized, atomic percentage of elements in fiber respectively. Catalytic activity was also measured.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Fundamental Electrochemistry, Technical University of Denmark
Authors: Marani, D. (Intern), Silva, R. H. (Ekstern), Zhang, W. (Intern), Werchmeister, R. M. L. (Intern), Kammer Hansen, K. (Intern), Esposito, V. (Intern)
Publication date: 2015
Event: Abstract from 1st Annual World Congress of Smart Materials 2015, Busan, Korea, Republic of.
Main Research Area: Technical/natural sciences
Source: PublicationPreSubmission
Source-ID: 106753942
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2015

Fabrication of Ni-5 at. %W Long Tapes with CeO2 Buffer Layer by Reel-to-Reel Method

A 10-m-long homemade textured Ni-5at.%W (Ni5W) long tape with a CeO2 buffer layer has been prepared successfully by means of rolling-assisted biaxially textured substrate (RABiTS) route followed by a chemical solution deposition method in a reel-to-reel manner. Globally, the Ni5W substrate and CeO2 film exhibit high homogeneity in terms of biaxial texture over the tape. The average values of full width at half maximum of in-plane and out-of-plane texture are 7.2° and 6.1° in Ni5W substrate, 7.6° and 6.1° in CeO2 buffer layer, respectively, all of those with a small standard deviation. On a microlevel, the CeO2 film epitaxially grows well on top of the Ni5W tape. A continuous, smooth, and crack-free morphology was observed on the CeO2 film and the fraction of low-angle grain boundaries (≤ 10°) is about 98 %. This process is a potential possibility for producing long-length textured CeO2/Ni5W tapes for coated conductors with a low cost.

General information
State: Published
Organisations: Electrofunctional materials, Department of Energy Conversion and Storage, Beijing University of Technology
Ni-5at.% W tapes, CeO2 buffer layer, Reel-to-reel, Long tape, Cube texture
Fabrication of porous 3-YSZ turbular supports for oxygen transport membranes

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, Ceramic Engineering & Science
Authors: Bjørnetun Haugen, A. (Intern), Gurauskis, J. (Intern), Ovtar, S. (Intern), Hendriksen, P. V. (Intern), Kaiser, A. (Intern)
Number of pages: 1
Publication date: 2015
Event: Abstract from Summer school on Ionic and protonic conducting ceramic membranes for green energy applications, Valencia, Spain.
Main Research Area: Technical/natural sciences
Electronic versions: Fabrication_of_porous.pdf

Bibliographical note
Poster presentation
Source: PublicationPreSubmission
Source-ID: 118022937
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2015

Fabrication of thin yttria-stabilized-zirconia dense electrolyte layers by inkjet printing for high performing solid oxide fuel cells

In this work, we present how a low-cost HP Deskjet 1000 inkjet printer was used to fabricate a 1.2 mm thin, dense and gas tight 16 cm² solid oxide fuel cells (SOFC) electrolyte. The electrolyte was printed using an ink made of highly diluted (<4 vol.%) nanometric yttria stabilized zirconia (YSZ) powders (50 nm in size) in an aqueous medium. The ink was designed to be a highly dispersed, long term stable colloidal suspension, with optimal printability characteristics. The electrolyte was made by a multiple printing procedure, which ensures coverage of the several flaws occurring in a single printing pass. Together with an optimized sintering procedure this resulted in good adhesion and densification of the electrolyte. The SOFC exhibited a close-to-theoretical open circuit voltage and a remarkable peak power density above 1.5 W cm⁻² at 800 °C.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Applied Electrochemistry , Fundamental Electrochemistry, Mixed Conductors
Pages: 89-95
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Power Sources
Volume: 273
ISSN (Print): 0378-7753
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 7 SJR 2.202 SNIP 1.536
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 6.22 SJR 1.944 SNIP 1.5
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.9 SNIP 1.667 CiteScore 6.34
Fast mass interdiffusion in ceria/alumina composite

Gadolinium-doped ceria (CGO) presents unique processes at low oxygen partial pressure (pO2 < 10^-12 atm) and low temperatures (T > 800 °C) such as faster mass diffusion, which are not observed in conventional sintering under ambient air conditions. In CGO/Al2O3 composites the resulting effects driven by such mass diffusion are low viscosity flows and high reactivity between phases, indicated by the formation of CeAlO3. This reaction is promoted by the high content of oxygen defects and the chemical reduction of Ce4+ cations to Ce3+ in CGO/Al2O3 composites under low temperature and low pO2. In this work, a comparison is made between sintering CGO/Al2O3 under ambient air conditions and under low pO2, focusing on densification, viscosity and the evolution of the microstructure.

General information
Fe\textsubscript{3}C-based oxygen reduction catalysts: synthesis, hollow spherical structures and applications in fuel cells

We present a detailed study of a novel Fe3C-based spherical catalyst with respect to synthetic parameters, nanostructure formation, ORR active sites and fuel cell demonstration. The catalyst is synthesized by high temperature autoclave pyrolysis using decomposing precursors. Below 500 °C, melamine-rich microspheres are first developed with uniformly dispersed amorphous Fe species. During the following pyrolysis at temperatures from 600 to 660 °C, a small amount of Fe3C phase with possible Fe–Nx/Cactive sites are formed, however, with moderate catalytic activity, likely limited by the low conductivity of the catalyst. At high pyrolytic temperatures of 700–800 °C, simultaneous formation of Fe3C nanoparticles and encasing graphitic layers occur within the morphological confinement of the microspheres. With negligible surface nitrogen or iron functionality, the thus-obtained catalysts exhibit superior ORR activity and stability. A new ORR active phase of Fe3C nanoparticles encapsulated by thin graphitic layers is proposed. The activity and durability of the catalysts are demonstrated in both Nafion-based low temperature and acid doped polybenzimidazole-based high temperature proton exchange membrane fuel cells.

Fe\textsubscript{x}C-based oxygen reduction catalysts: synthesis, hollow spherical structures and applications in fuel cells

We present a detailed study of a novel Fe3C-based spherical catalyst with respect to synthetic parameters, nanostructure formation, ORR active sites and fuel cell demonstration. The catalyst is synthesized by high temperature autoclave pyrolysis using decomposing precursors. Below 500 °C, melamine-rich microspheres are first developed with uniformly dispersed amorphous Fe species. During the following pyrolysis at temperatures from 600 to 660 °C, a small amount of Fe3C phase with possible Fe–Nx/Cactive sites are formed, however, with moderate catalytic activity, likely limited by the low conductivity of the catalyst. At high pyrolytic temperatures of 700–800 °C, simultaneous formation of Fe3C nanoparticles and encasing graphitic layers occur within the morphological confinement of the microspheres. With negligible surface nitrogen or iron functionality, the thus-obtained catalysts exhibit superior ORR activity and stability. A new ORR active phase of Fe3C nanoparticles encapsulated by thin graphitic layers is proposed. The activity and durability of the catalysts are demonstrated in both Nafion-based low temperature and acid doped polybenzimidazole-based high temperature proton exchange membrane fuel cells.
Fine structure of modal focusing effect in a three dimensional plasma-sheath-lens formed by disk electrodes

Modal and discrete focusing effects associated with three-dimensional plasma-sheath-lenses show promising potential for applications in ion beam extraction, mass spectrometry, plasma diagnostics and for basic studies of plasma sheath. The ion focusing properties can be adjusted by controlling the geometrical structure of the plasma-sheath-lens and plasma parameters. The positive and negative ion kinetics within the plasma-sheath-lens are investigated both experimentally and theoretically and a modal focusing ring is identified on the surface of disk electrodes. The focusing ring is very sensitive to the sheath thickness and can be used to monitor very small changes in plasma parameters. Three dimensional simulations are found to be in very good agreement with experiments.
First principles investigation of the activity of thin film Pt, Pd and Au surface alloys for oxygen reduction

Further advances in fuel cell technologies are hampered by kinetic limitations associated with the sluggish cathodic oxygen reduction reaction. We have investigated a range of different formulations of binary and ternary Pt, Pd and Au thin films as electrocatalysts for oxygen reduction. The most active binary thin films are near-surface alloys of Pt with subsurface Pd and certain PdAu and PtAu thin films with surface and/or subsurface Au. The most active ternary thin films are with pure metal Pt or Pd skins with some degree of Au in the surface and/or subsurface layer and the near-surface alloys of Au with mixed Pt/Pd skins. The activity of the binary and ternary catalysts is explained through weakening of the OH binding energy caused by solute elements. However, given the low alloy formation energies it may be difficult to tune and retain the composition under operating conditions. This is particularly challenging for alloys containing Au due to a high propensity of Au to segregate to the surface. We also show that once Au is on the surface it will diffuse to defect sites, explaining why small amounts of Au retard dissolution of Pt nanoparticles. For the PtPd thin films there is no pronounced driving force for surface segregation, diffusion to defects or surface self-assembling. On the basis of stability and activity analysis we conclude that the near surface alloy of Pd in Pt and some PdAu binary and PtPdAu ternary thin films with a controlled amount of Au are the best catalysts for oxygen reduction.
Flexible sample environment for high resolution neutron imaging at high temperatures in controlled atmosphere

High material penetration by neutrons allows for experiments using sophisticated sample environments providing complex conditions. Thus, neutron imaging holds potential for performing in situ nondestructive measurements on large samples or even full technological systems, which are not possible with any other technique. This paper presents a new sample environment for in situ high resolution neutron imaging experiments at temperatures from room temperature up to 1100 °C and/or using controllable flow of reactive atmospheres. The design also offers the possibility to directly combine imaging with diffraction measurements. Design, special features, and specification of the furnace are described. In addition, examples of experiments successfully performed at various neutron facilities with the furnace, as well as examples of possible applications are presented. This covers a broad field of research from fundamental to technological investigations of various types of materials and components. © 2015 AIP Publishing LLC.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Imaging and Structural Analysis, Proton conductors, Xnovo Technology ApS, Oak Ridge National Laboratory, University of California at Berkeley, Karlsruhe Institute of Technology KIT, Paul Scherrer Institut, European Spallation Source ESS AB, Rutherford Appleton Laboratory
Authors: Makowska, M. G. (Intern), Kuhn, L. T. (Intern), Cleemann, L. N. (Intern), Lauridsen, E. M. (Ekstern), Bilheux, H. Z. (Ekstern), Molaison, J. J. (Ekstern), Santodonato, L. J. (Ekstern), Tremsin, A. S. (Ekstern), Grosse, M. (Ekstern), Morgano, M. (Ekstern), Kabra, S. (Ekstern), Strobl, M. (Ekstern)

Bibliographical note
This article is published Open Access as part of the RSC's Gold for Gold initiative, licensed under a Creative Commons Attribution 3.0 Unported Licence.

Publication: Research - peer-review › Journal article – Annual report year: 2015
Fullerene alloy formation and the benefits for efficient printing of ternary blend organic solar cells

Composition average dependent properties for blends of the conjugated polymer P3HT and the fullerenes [60]PCBM, [60]CBA and their mixtures were studied using cross-polarization magic-angle-spinning solid-state NMR techniques. We found that the blended fullerenes form an alloy and that when mixed with a third polymer component, the system exhibits pseudo-binary phase behaviour instead of the expected ternary phase behaviour. Our results experimentally confirm the earlier hypothesis that the unexpected composition average dependent IV-behaviour for these supposed ternary mixtures are indeed due to them behaving as pseudo-binary mixtures due to alloying of the fullerene components. This finding has vast implications for the understanding of polymer–fullerene mixtures and quite certainly also their application in organic solar cells where performance hinges critically on the blend behaviour which is also investigated in this study.

General information

State: Published
Organisations: Department of Energy Conversion and Storage, Functional organic materials, Aarhus University, University of Southern California
Authors: Angmo, D. (Intern), Bjerring, M. (Ekstern), Nielsen, N. C. (Ekstern), Thompson, B. C. (Ekstern), Krebs, F. C. (Intern)
Number of pages: 8
Pages: 5541-5548
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information

Journal: Journal of Materials Chemistry C
Volume: 3
Issue number: 21
ISSN (Print): 2050-7526
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 1.3 SJR 1.917 CiteScore 5.67
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 5.14 SJR 1.825 SNIP 1.266
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.713 SNIP 1.508 CiteScore 5.32
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.517 SNIP 1.351 CiteScore 4.64
Web of Science (2014): Indexed yes
Functional Analysis of Battery Management Systems using Multi-Cell HIL Simulator

Developers and manufacturers of Battery Management Systems (BMSs) require extensive testing of controller HW and SW, such as analog front-end (AFE) and performance of generated control code. In comparison with tests conducted on real batteries, tests conducted on hardware-in-the-loop (HIL) simulator may be more costant time effective, easier to reproduce and safer beyond the normal range of operation, especially at early stages in the development process or during fault simulation. In this paper a li-ion battery (LIB) electro-thermal multicell model coupled with an aging model is designed, characterized and validated based on experimental data, converted to C code and emulated in real-time with a dSpace HIL simulator. The BMS to be tested interacts with the emulated battery pack as if it was managing a real battery pack. BMS functions such as protection, measuring of current, voltage and temperature or balancing are tested on real-time experiments.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, Aalborg University, RWTH Aachen University
Authors: Barreras, J. V. (Ekstern), Swierczynski, M. J. (Ekstern), Schaltz, E. (Ekstern), Andreasen, S. J. (Ekstern), Fleischer, C. (Ekstern), Sauer, D. U. (Ekstern), Christensen, A. E. (Intern)
Number of pages: 10
Publication date: 2015

Host publication information
Title of host publication: Proceedings of the 2015 Tenth International Conference on Ecological Vehicles and Renewable Energies (EVER)
Publisher: IEEE
ISBN (Print): 978-1-4673-6784-4
Main Research Area: Technical/natural sciences
Conference: 10th International Conference on Ecological Vehicles and Renewable Energies, Monte-Carlo, Monaco, 31/03/2015 - 31/03/2015
Battery management system, Hardware-in-the-loop, Lithium ion
DOIs:
10.1109/ever.2015.7112984
Source: FindIt
Source-ID: 2287529050
Publication: Research - peer-review › Article in proceedings – Annual report year: 2015

Functionally Graded Ceramics Fabricated with Side-by-Side Tape Casting for Use in Magnetic Refrigeration

Functionally graded ceramic tapes have been fabricated by a side-by-side tape casting technique. This study shows the possibility and describes the main principles of adjacent coflow of slurries resulting in formation of thin plates of graded ceramic material. Results showed that the small variations of solvent and binder system concentrations have a substantial effect on slurry viscosity. Varying these parameters showed that side-by-side tape casting with a well-defined interface area is possible for slurries with viscosities above 3500 mPa s at a casting shear rate of 3.3 s⁻¹. As it was expected, the choice of de-bindering and sintering regimes significantly influences crack formation, and a three-step heating programme was found to result in tapes of the highest quality. The interface regions of green graded tapes were investigated structurally by scanning electron microscopy; for a distinct identification of the interface region and analysing the degree of cross-interface diffusion, the isothermal entropy change was measured by a vibrating sample magnetometer as the magnetic transition temperature (Curie temperature) is very sensitive to the dopant level in ceramics. Also the purpose of developing this graded ceramic tape casting was applications of these specific magnetocaloric properties within the magnetic refrigeration technology.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Electrofunctional materials, Imaging and Structural Analysis
Authors: Bulatova, R. (Intern), Bahl, C. (Intern), Andersen, K. B. (Intern), Kuhn, L. T. (Intern), Pryds, N. (Intern)
Number of pages: 8
Fundamental electrochemistry: general discussion

State: Published
Organisations: Department of Energy Conversion and Storage, Fundamental Electrochemistry, Applied Electrochemistry
Number of pages: 36
Pages: 177-212
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Faraday Discussions
Volume: 182
ISSN (Print): 1359-6640
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
Fundamental mechanisms in Li-air battery electrochemistry

The lithium-air (or Li-O2) batteries have received wide attention as an enabling technology for a mass market entry of electric vehicles due to a potential capacity much higher than current Li-ion technology. The technology is a relatively new battery concept proposed in 1996, and the current research still focuses on developing an understanding of the reactions inside the battery. This thesis is dedicated to increase this understanding and use the knowledge to improve the performance of the battery, and the work span from detailed investigation of the atom positions to the proposal of a system used to manage a full size electric vehicle battery. An automated differential electrochemical mass spectrometer (DEMS) was built to investigate the relationship between current and the consumption and release of gases, which is important to
identify and quantify degradation reactions. The setup was used to characterize our carbon-based reference system as well as new ionic liquid-based electrolytes. Electrochemical impedance spectroscopy (EIS) has been used extensively to describe reaction mechanisms inside the battery; the origin of the measured overpotentials; and the onset potential for electrochemical degradation. It was confirmed that the rapid potential loss near the end of discharge could be explained by an increase in the charge transport resistance; that the initial Li2O2 oxidation at 3.05 V was blocked by the formation of an SEI layer; and that the voltage increase during charge was primarily due to the formation of a mixed potential between competing oxidation reactions needed to maintain a constant current. The knowledge about impedance spectroscopy was used to propose and investigate a novel battery management tool to estimate the state of charge and the state of health of a Li-O2 battery system better than any other method available. Finally, calculations were made to support that an open system configuration is a realistic option in terms of air purification, if H2O and CO2 levels at 1 ppm are allowed.

**General information**

*State:* Published  
*Organisations:* Department of Energy Conversion and Storage, Atomic scale modelling and materials, Haldor Topsoe AS  
*Authors:* Højberg, J. (Intern), Vegge, T. (Intern), Norby, P. (Intern), Johansen, K. (Ekstern)  
*Number of pages:* 199  
*Publication date:* 2015

**Publication information**

*Publisher:* Department of Energy Conversion and Storage, Technical University of Denmark  
*Original language:* English  
*Main Research Area:* Technical/natural sciences  
*Electronic versions:*  
*PhD_Thesis_20150520_rev1_til_Orbit.pdf*  
*Publication:* Research › Ph.D. thesis – Annual report year: 2015

**Graphene oxide and hyperbranched polymer-toughened hydrogels with improved absorption properties and durability**

Hyperbranched polymers or graphene oxide nanosheets were used to synthesize poly(acrylic acid)-based hybrid hydrogels with high water absorption ability, excellent mechanical properties, and environmental remediation abilities through a novel one-step, cost-effective, and environmentally friendly method. The combination of hyperbranched polymers and graphene oxide nanosheets had synergistic effects on the final hybrid hydrogel, especially on the mechanical behaviors of the hydrogels, with Young's modulus, tensile strength at break and elongation at break increasing by 69, 308, and 848 %, respectively, while the other properties remained similar to those of pure poly(acrylic acid). The proposed enhancement mechanism is also discussed.

**General information**

*State:* Published  
*Organisations:* Department of Energy Conversion and Storage, Ceramic Engineering & Science, Flinders University, South China University of Technology, University of South Australia  
*Authors:* Yu, Y. (Ekstern), De Andrade, L. C. X. (Ekstern), Fang, L. (Ekstern), Ma, J. (Ekstern), Zhang, W. (. (Intern), Tang, Y. (Ekstern))  
*Number of pages:* 10  
*Pages:* 3457-3466  
*Publication date:* 2015  
*Main Research Area:* Technical/natural sciences

**Publication information**

*Journal:* Journal of Materials Science  
*Volume:* 50  
*Issue number:* 9  
*ISSN (Print):* 0022-2461  
*Ratings:*  
*BFI (2018):* BFI-level 1  
*Web of Science (2018):* Indexed yes  
*BFI (2017):* BFI-level 1  
*Scopus rating (2017):* SNIP 1.064 SJR 0.807 CiteScore 2.83  
*Web of Science (2017):* Indexed yes  
*BFI (2016):* BFI-level 1  
*Scopus rating (2016):* CiteScore 2.49 SJR 0.769 SNIP 1.072  
*Web of Science (2016):* Indexed yes  
*BFI (2015):* BFI-level 1  
*Scopus rating (2015):* SJR 0.792 SNIP 1.059 CiteScore 2.36  
*Web of Science (2015):* Indexed yes
Growth of Highly Epitaxial \(\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}\) Films from a Simple Propionate-Based Solution

Intensive investigations have been conducted to develop epitaxial oxide thin films with superior electromagnetic performance by low-cost chemical solution deposition routes. In this paper, a novel propionate-based precursor solution
without involving any other additive was proposed and employed to grow superconducting YBa2Cu3O7-δ (YBCO) films on LaAlO3 (LAO) single crystals. The precursor solutions are stable with a long shelf life of up to several months. Since the primary compositions are propionates after evaporating the solvent, the toxic reagents and evolved gases during solution synthesis and heat treatment can be eliminated completely. In this process, rapid pyrolysis and high conversation rate can also be achieved during growth of YBCO films in comparison with the conventional trifluoroacetate metal organic deposition routes. Remarkably, a 210 nm YBCO film exhibits high superconducting performance with a Jc value of 3.7 MA/cm(2) at 77 K, self-field. Nucleation and growth behaviors in the chemical solution process have also been studied. It is revealed that the amount of liquid phase (Ba-Cu-O) is sufficient through the entire thickness within a very short time at high growth temperatures, which results in pronounced densification and fast conversion of the YBCO phase.

**General information**

State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, Electrofunctional materials, Universidad Autonoma de Barcelona, University of Hamburg
Authors: Yue, Z. (Intern), Torres, P. (Ekstern), Tang, X. (Ekstern), Norby, P. (Intern), Grivel, J. (Intern)
Number of pages: 7
Pages: 10232–10238
Publication date: 2015
Main Research Area: Technical/natural sciences

**Publication information**

Journal: Inorganic Chemistry
Volume: 54
Issue number: 21
ISSN (Print): 0020-1669
Ratings:
- BFI (2018): BFI-level 2
- Web of Science (2018): Indexed yes
- BFI (2017): BFI-level 2
- Scopus rating (2017): CiteScore 4.7 SJR 1.892 SNIP 1.123
- Web of Science (2017): Indexed Yes
- BFI (2016): BFI-level 2
- Scopus rating (2016): CiteScore 4.64 SJR 1.804 SNIP 1.199
- Web of Science (2016): Indexed yes
- BFI (2015): BFI-level 2
- Scopus rating (2015): SJR 1.782 SNIP 1.229 CiteScore 4.7
- Web of Science (2015): Indexed yes
- BFI (2014): BFI-level 2
- Scopus rating (2014): SJR 1.867 SNIP 1.306 CiteScore 4.69
- Web of Science (2014): Indexed yes
- BFI (2013): BFI-level 2
- Scopus rating (2013): SJR 1.821 SNIP 1.368 CiteScore 4.9
- ISI indexed (2013): ISI indexed yes
- Web of Science (2013): Indexed yes
- BFI (2012): BFI-level 2
- Scopus rating (2012): SJR 2.094 SNIP 1.341 CiteScore 4.72
- ISI indexed (2012): ISI indexed yes
- Web of Science (2012): Indexed yes
- BFI (2011): BFI-level 2
- Scopus rating (2011): SJR 1.921 SNIP 1.313 CiteScore 4.64
- ISI indexed (2011): ISI indexed yes
- Web of Science (2011): Indexed yes
- BFI (2010): BFI-level 2
- Scopus rating (2010): SJR 2.006 SNIP 1.309
- Web of Science (2010): Indexed yes
- BFI (2009): BFI-level 2
- Scopus rating (2009): SJR 2.014 SNIP 1.528
- Web of Science (2009): Indexed yes
H/D isotope effects in high temperature proton conductors

The atomic mass ratio of ca. 2 between deuterium and hydrogen is the highest for any pair of stable isotopes and results in significant and measurable H/D isotope effects in high temperature proton conductors containing these species. This paper discusses H/D isotope effects manifested in O-H/O-D vibration frequencies, the mobility of H⁺/D⁺ carriers, the kinetics of the electrochemical oxidation of H₂/D₂, the solubilities of H₂O/D₂O and, finally, the spontaneous electromotive force that appears across H₂/D₂ cells with proton conducting electrolytes. Comparable work on tritium-exchanged materials is also discussed. The results highlight the usefulness of isotope effects in the study of high temperature proton conductors.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Mixed Conductors, University of Twente
Authors: Bonanos, N. (Intern), Huijser, A. (Ekstern), Poulsen, F. W. (Intern)
Number of pages: 5
Pages: 9-13
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Solid State Ionics
Volume: 275
ISSN (Print): 0167-2738
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 2.64 SJR 0.856 SNIP 0.952
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.41 SJR 0.75 SNIP 0.909
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.802 SNIP 1.016 CiteScore 2.5
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.837 SNIP 1.282 CiteScore 2.62
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.903 SNIP 1.269 CiteScore 2.35
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.051 SNIP 1.253 CiteScore 2.31
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.376 SNIP 1.615 CiteScore 2.96
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.46 SNIP 1.498
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.508 SNIP 1.483
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.515 SNIP 1.617
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.292 SNIP 1.384
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.239 SNIP 1.541
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.093 SNIP 1.423
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.18 SNIP 1.55
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.473 SNIP 1.389
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 1.253 SNIP 1.36
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 1.121 SNIP 1.213
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 1.161 SNIP 1.312
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 1.08 SNIP 1.254
Original language: English
Proton conductor Isotope effect Hydrogen Deuterium Tritium Zero point energy, Carrier mobility, Deuterium, Electrochemical oxidation, Hydrogen, Protons, Tritium, Atomic mass, High temperature proton conductor, Isotope effect, Proton conductors, Proton-conducting electrolyte, Stable isotopes, Vibration frequency, Zero-point energies, Isotopes
Electronic versions:
H_D_Isotope_Effects_in_High_Temperature_Proton_Conductors_postprint.pdf. Embargo ended: 06/04/2017
DOIs:
10.1016/j.ssi.2015.03.028
Source: FindIt
Source-ID: 274817742
Publication: Research - peer-review › Journal article – Annual report year: 2015
High-Jc YBa2Cu3O7−x−Ag superconducting thin films synthesized through a fluorine-free MOD method

Obtaining a high critical current density (Jc) remains the main challenge in developing fluorine-free metal organic deposition (MOD) methods to fabricate YBCO superconducting thin films. Silver addition was used to raise the Jc values in this research work. By reacting with propionic acid and ammonia, AgNO3 was initially mixed with YBCO carboxylate precursors dissolved in methanol. High-temperature in situ XRD measurements on the YBCO-Ag powders revealed that silver addition lowers the incongruent melting temperature of YBCO to 760°C and resulted in a smooth surface morphology of the YBCO films at a temperature as low as 760°C. Grain growth and intergranular conductivity were also found to be improved by silver doping. After annealing under optimized conditions, a high Jc of 4.6 MA/cm² was obtained in a YBCO-Ag thin film with 10 wt% Ag.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Department of Physics, Neutrons and X-rays for Materials Physics, Tsinghua University
Authors: Tang, X. (Intern), Yue, Z. (Intern), Wu, W. (Ekstern), Grivel, J. (Intern), Andersen, N. H. (Intern)
Pages: 1761−1769
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of the European Ceramic Society
Volume: 35
Issue number: 6
ISSN (Print): 0955-2219
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 3.55 SJR 1.068 SNIP 1.698
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.25 SJR 1.142 SNIP 1.888
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.135 SNIP 1.817 CiteScore 3.03
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.163 SNIP 2.083 CiteScore 3.16
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.111 SNIP 1.79 CiteScore 2.57
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.293 SNIP 2.207 CiteScore 2.81
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.343 SNIP 2.195 CiteScore 2.83
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.383 SNIP 1.93
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.374 SNIP 1.712
Highly Confined Electronic and Ionic Conduction in Oxide Heterostructures

The conductance confined at the interface of complex oxide heterostructures provides new opportunities to explore nanoionic devices. In this talk I will present our recent results both on ionic and electronic conductivity at different heterostructures systems. In the first part of my talk I will show some of our resent results that we demonstrated the possibility of stabilizing $\delta$-Bi$_2$O$_3$ using highly coherent interfaces of alternating layers. Remarkably, an exceptionally high chemical stability in reducing conditions and redox cycles at high temperature, usually unattainable for Bi$_2$O$_3$-based materials, is achieved[1]. These confined heterostructures provide a playground not only for new high ionic conductivity phenomena that are sufficiently stable but also uncover a large variety of possible technological perspectives. At the second part, I will discuss and show our recent results of high mobile samples realized by, interface confined redox reactions[2], strain induced polarization[3]and modulation doping at complex oxide interfaces. This collection of samples offers unique opportunities for a wide range of rich world of mesoscopic physics.

High performance p-type segmented leg of misfit-layered cobaltite and half-Heusler alloy

In this study, a segmented p-type leg of doped misfit-layered cobaltite $\text{Ca}_{2.8}\text{Lu}_{0.15}\text{Ag}_{0.05}\text{Co}_4\text{O}_9+\delta$ and half-Heusler $\text{Ti}_{0.3}\text{Zr}_{0.35}\text{Hf}_{0.35}\text{Co}_8\text{Sb}_{0.8}\text{Sn}_{0.2}$ alloy was fabricated and characterized. The thermoelectric properties of single components, segmented leg, and the electrical contact resistance of the joint part were measured as a function of temperature. The output power generation characteristics of segmented legs were characterized in air under various temperature gradients, $\Delta T$, with the hot side temperature up to 1153 K. At $\Delta T \approx 756$ K, the maximum conversion efficiency reached a value of $\sim 5\%$, which is about 65% of that expected from the materials without parasitic losses. The long-term stability investigation for two weeks at the hot and cold side temperatures of 1153/397 K shows that the segmented leg has good durability as a result of stable and low electrical resistance contacts. 2015 Elsevier Ltd. All rights reserved.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, North Carolina State University, California Institute of Technology, Johannes Gutenberg University
Authors: Le, T. H. (Intern), Van Nong, N. (Intern), Snyder, G. J. (Ekstern), Viet, M. H. (Ekstern), Balke, B. (Ekstern), Han, L. (Intern), Stamate, E. (Intern), Linderoth, S. (Intern), Pryds, N. (Intern)
Pages: 20–27
Publication date: 2015
Main Research Area: Technical/natural sciences
High performing SOFC via multilayer tape casting?

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry
Authors: Hauch, A. (Intern)
Publication date: 2015
Main Research Area: Technical/natural sciences
Electronic versions:
EFCF_poster_cbir_2012_06_22_hauc_edit_FINAL.pdf

Relations
Activities:
European Fuel Cell Forum 2012
Publication: Research - peer-review › Poster – Annual report year: 2015

High Temperature Electrolysis
High temperature electrolysis of carbon dioxide, or co-electrolysis of carbon dioxide and steam, has a great potential for carbon dioxide utilisation. A solid oxide electrolysis cell (SOEC), operating between 500 and 900 °C, is used to reduce carbon dioxide to carbon monoxide. If steam is also input to the cell then hydrogen is produced giving syngas. This syngas can then be further reacted to form hydrocarbon fuels and chemicals. Operating at high temperature gives much higher efficiencies than can be achieved with low temperature electrolysis. Current state of the art SOECs utilise a dense electrolyte, commonly yttria-stabilised-zirconia (YSZ), with porous fuel and oxygen side electrodes. The electrodes must be both electron and oxide ion conducting, and maximising the active surface area is essential for efficient operation. For the fuel electrode a cermet of nickel and YSZ is often used, whereas a lanthanum strontium manganite - YSZ mix is utilised for the oxygen electrode. Long term durability and performance are key for commercialisation of SOEC technology. To date, experimental tests of 1000 h on electrolysis stacks operated at low current density have shown little or no degradation when inlet gas cleaning is employed; however, operation at higher current density leads to cell degradation, which still needs to be overcome. Advances in materials and morphology are needed to further decrease cell degradation.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Fundamental Electrochemistry, University of Sheffield
High-temperature stability of thermoelectric Ca$_3$Co$_4$O$_9$ thin films

An enhanced thermal stability in thermoelectric Ca$_3$Co$_4$O$_9$ thin films up to 550 °C in an oxygen rich environment was demonstrated by high-temperature electrical and X-ray diffraction measurements. In contrast to generally performed heating in helium gas, it is shown that an oxygen/helium mixture provides sufficient thermal contact, while preventing the previously disregarded formation of oxygen vacancies. Combining thermal cycling with electrical measurements proves to be a powerful tool to study the real intrinsic thermoelectric behaviour of oxide thin films at elevated temperatures. © 2015 AIP Publishing LLC.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, University of Twente
Authors: Brinks, P. (Ekstern), Van Nong, N. (Intern), Pryds, N. (Intern), Rijnders, G. (Ekstern), Huijben, M. (Ekstern)
Number of pages: 4
Publication date: 2015
Main Research Area: Technical/natural sciences
Publication information
Volume: 106
Article number: 143903
ISSN (Print): 0003-6951
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 3.25 SJR 1.382 SNIP 1.167
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.67 SJR 1.673 SNIP 1.249
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.499 SNIP 1.226 CiteScore 2.47
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.861 SNIP 1.492 CiteScore 3.25
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.146 SNIP 1.633 CiteScore 3.77
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 2.57 SNIP 1.739 CiteScore 3.76
ISI indexed (2012): ISI indexed yes
Hybrid direct carbon fuel cell anode processes investigated using a 3-electrode half-cell setup
A 3-electrode half-cell setup consisting of a yttria-stabilized zirconia (YSZ) electrolyte support was employed to investigate the chemical and electrochemical processes occurring in the vicinity of a model hybrid direct carbon fuel cell (HDCFC) anode (Ni-YSZ) in contact with a molten carbon-alkali carbonate slurry. Electrochemical testing, cyclic voltammetry (CV) and electrochemical impedance spectroscopy (EIS), with and without the Ni-YSZ layer highlighted the promotional effect of the Ni-YSZ anode layer, and revealed the contributions of Ni/NiO, and potentially K/K2O, redox couple(s). Treated anthracite and bituminous coals, as well as carbon black, were tested, revealing similar open circuit potential and activation energies in mixed 96-4vol% N2-CO2 and 50-50vol% CO-CO2 environments between 700 and 800°C. Bituminous coal showed the highest activity, likely associated to a high O/C ratio and hydrogen content. Based on acquired data, a reaction scheme was proposed for processes at the working electrode, including the role of bubble formation in the vicinity of the electrochemically active solid/molten medium interface.
Hybrid Direct Carbon Fuel Cell Performance with Anode Current Collector Material

The influence of the current collector on the performance of a hybrid direct carbon fuel cell (HDCFC), consisting of solid oxide fuel cell (SOFC) with a molten carbonate-carbon slurry in contact with the anode, has been investigated using current-voltage curves. Four different anode current collectors were studied: Au, Ni, Ag, and Pt. It was shown that the performance of the direct carbon fuel cell (DCFC) is dependent on the current collector materials, Ni and Pt giving the best performance, due to their catalytic activity. Gold is suggested to be the best material as an inert current collector, due to its low catalytic activity.
Hybrid TEG-heat exchanger module for electrical power production

**General information**

**State:** Published

**Organisations:** Department of Energy Conversion and Storage, Electrofunctional materials

**Authors:** Sarhadi, A. (Intern), Bjørk, R. (Intern), Nielsen, K. K. (Intern), Pryds, N. (Intern)

**Number of pages:** 1

**Publication date:** 2015

**Event:** Abstract from 34th Annual International Conference on Thermoelectrics (ICT 2015) and 13th European conference on Thermoelectrics (ECT 2015), Dresden, Germany.

**Main Research Area:** Technical/natural sciences

**Electronic versions:**

Hybrid_TEG_heat_exchanger.pdf

**Source:** PublicationPreSubmission

**Source-ID:** 117916251

**Publication:** Research - peer-review › Conference abstract for conference – Annual report year: 2015

---

Hydrogen Energy by Means of Proton Conductors

If we dare to take serious what we know today about climate issues the challenges to our energy systems are immense. If we really chose - also in practice - to phase out the fossil fuels major changes to the way we handle energy are required. The renewable energy resources are by far sufficient, but matching supply and demand in time as well as in form calls for new engineering solutions. Hydrogen as energy carrier and energy storage medium has often been mentioned as an option for the future. A proton is an elementary particles, but at the same time the ion of hydrogen. When hydrogen (H2) is extracted from water (H2O) it can happen via formation of protons (hydrogen ions, H+) which must be transported away by proton conducting materials to form molecular hydrogen (H2). This process is called electrolysis and converts electrical energy into the chemical energy of a fuel. The reverse process of making electricity from a fuel takes place in a fuel cell. The talk will present different aspects of the concept of hydrogen energy and how materials science can bring this technology of the future closer to the present.

**General information**

**State:** Published

**Organisations:** Department of Energy Conversion and Storage, Proton conductors

**Authors:** Jensen, J. O. (Intern)

**Publication date:** 2015

**Event:** Abstract from Tiltrædelsesforelæsning, Lyngby, Denmark.

**Main Research Area:** Technical/natural sciences

**Bibliographical note**

Inaugural Lecture (Professor)

**Source:** PublicationPreSubmission

**Source-ID:** 127806504

**Publication:** Communication › Conference abstract for conference – Annual report year: 2016
Identifying Activity Descriptors for CO2 Electro-Reduction to Methanol on Rutile (110) Surfaces

Electrocatalytic reduction of CO2 to liquid fuels using energy from renewable sources has the potential to form the basis of a carbon neutral sustainable energy system, while integrating seamlessly in the established infrastructure. Storing intermittent renewable energy in a chemical fuel is especially attractive to achieve high energy density required for transport applications. Among the metals, Cu electrocatalyst can convert CO2 to methane and ethylene in aqueous electrolytes at ambient temperature with moderate efficiency. However, a high overpotential is required for this reaction and almost no alcohols are produced. Experimental studies have shown that mixed rutile oxides (Ru/Ir/Ti) can catalyze the conversion of CO2 to alcohols. However, very little is known about the reduction of CO2to alcohols on oxide electrocatalysts. Here, we present a computational study of the thermo-dynamics of the 6e- reduction of CO2 to methanol on substituted RuO2 (110) surfaces. We replace the Ru atoms in top layer with ten other transition metals, which in their +4 oxidation state have ionic radius comparable to Ru in octahedral coordination. The substituted surfaces show large variations in surface reactivity enabling us to explore the reduction of CO2to methanol in a wide materials window. We use the computational hydrogen electrode model to calculate the potential dependent reaction free energies from density functional theory based calculations using BEEF-vdW functional and PAW method as implemented in VASP. We consider corrections for zero point energy, heat capacity, entropic contribution and other energy correction for CO2 and H2 molecule. The simulation model employs ¼ monolayer of CO coverage as spectator species to emulate the presence of CO produced simultaneously by reduction of CO2. We show the electronic binding energies for reduction intermediates such as O, OCHO, HCOOH, and H2COOH scale linearly with that of OH on partially CO covered, reduced rutile surfaces. This scaling can be rationalized, by the fact all these adsorbates bind to the surfaces through the oxygen atoms. This enables us to describe the theoretical electrochemical potential required to drive the reaction as a function of the OH binding energy. Considering the OH binding energy as the prime descriptor, we can establish a volcano plot for this reaction (Figure 1). For surfaces binding OH very strongly e.g. Nb, removal of OH from active site is the most endergonic step. On the contrary, surfaces binding OH weakly e.g. Pd will need large reducing potential to protonate HCOOH to methanol. While surfaces with Ir, Sn or Pt have optimal OH binding energy, for efficient methanol production, it is also important the HCOOH intermediate is bound sufficiently strongly to be further reduced to methanol. A third condition is to increase the overpotential for the parasitic production of hydrogen as much as possible. These parameters are also considered in order to evaluate the suitability of the substituted surfaces towards electrocatalytic production of methanol. We would like to acknowledge the Lundbeck Foundation for financial support of this work. References: 1. Lewis, N. S. & Nocera, D. G. Powering the planet: chemical challenges in solar energy utilization. Proc. Natl. Acad. Sci. U. S. A.103,15729–35 (2006). doi: 10.1073/pnas.0603395103 2. Y. Hori. Electrochemical CO2 reduction on metal electrodes, in Modern Aspects of Electrochemistry, Vol. 42, chapter 3, pp. 89–189, Springer, New York, 2008 3. Popic, J. P., Avramovic, M. L. & Vukovic, N. B. Reduction of carbon dioxide on ruthenium oxide and modified ruthenium oxide electrodes in 0.5 M NaHCO3. 421,(1997). doi:10.1016/S0022-0728(96)04823-1 4. Qu, J., Zhang, X., Wang, Y. & Xie, C. Electrochemical reduction of CO2 on RuO2/TiO2 nanotubes composite modified Pt electrode. Electrochim. Acta 50,3576–3580 (2005). doi:10.1016/j.electacta.2004.11.061 5. Ullah, N., Ali, I., Jansen, M. & Omanovic, S. Electrochemical reduction of CO in an aqueous electrolyte employing an iridium/ruthenium-oxide electrode. Can. J. Chem. Eng. (2014). doi:10.1002/cjce.22110 6. Nørskov, J. K. et al. Origin of the Overpotential for Oxygen Reduction at a Fuel-Cell Cathode. J. Phys. Chem. B108,17886–17892 (2004). doi: 10.1021/jp047349j 7. Chan, K., Tsai, C., Hansen, H. A. & Nørskov, J. K. Molybdenum Sulfides and Selenides as Possible Electrocatalysts for CO2 Reduction. ChemCatChem,6, (2014) doi: 10.1002/cctc.201402128 Figure 1: Theoretical activity volcano as a function of the OH binding energy on substituted surfaces. The line is drawn to guide the eye. Atomistic structure of the iridium substituted system is given. [Figure]
Identifying systematic DFT errors in catalytic reactions

Using CO2 reduction reactions as examples, we present a widely applicable method for identifying the main source of errors in density functional theory (DFT) calculations. The method has broad applications for error correction in DFT calculations in general, as it relies on the dependence of the applied exchange–correlation functional on the reaction energies rather than on errors versus the experimental data. As a result, improved energy corrections can now be determined for both gas phase and adsorbed reaction species, particularly interesting within heterogeneous catalysis. We show that for the CO2 reduction reactions, the main source of error is associated with the C–O bonds and not the typically energy corrected OCO backbone.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials
Authors: Christensen, R. (Intern), Hansen, H. A. (Intern), Vegge, T. (Intern)
Number of pages: 4
Pages: 4946-4949
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Catalysis Science & Technology
Volume: 5
Issue number: 11
ISSN (Print): 2044-4753
Ratings:
  BFI (2018): BFI-level 2
  Web of Science (2018): Indexed yes
  BFI (2017): BFI-level 1
  Scopus rating (2017): CiteScore 5.47 SJR 1.797 SNIP 1.149
  Web of Science (2017): Indexed Yes
  BFI (2016): BFI-level 1
  Scopus rating (2016): CiteScore 5.64 SJR 1.811 SNIP 1.287
  Web of Science (2016): Indexed yes
  BFI (2015): BFI-level 1
  Scopus rating (2015): SJR 1.804 SNIP 1.314 CiteScore 5.46
  Web of Science (2015): Indexed yes
  BFI (2014): BFI-level 1
  Scopus rating (2014): SJR 1.885 SNIP 1.47 CiteScore 5.44
  Web of Science (2014): Indexed yes
  BFI (2013): BFI-level 1
  Scopus rating (2013): SJR 1.744 SNIP 1.296 CiteScore 4.89
  ISI indexed (2013): ISI indexed yes
  Web of Science (2013): Indexed yes
  Scopus rating (2012): SJR 1.595 SNIP 1.036 CiteScore 3.7
  ISI indexed (2012): ISI indexed no
  ISI indexed (2011): ISI indexed no
Original language: English
Electronic versions: Identifying_systematic_DFT.pdf
DOIs: 10.1039/c5cy01332a

Bibliographical note
This article is published Open Access as part of the RSC's Gold for Gold initiative, licensed under a Creative Commons Attribution 3.0 Unported Licence.

Relations
Activities:
Improved Accuracy of Density Functional Theory Calculations for CO2 Reduction and Metal-Air Batteries
Source: FindIt
Source-ID: 2281738818
Publication: Research - peer-review → Journal article – Annual report year: 2015
Impedance-Based Battery Management for Metal-O2 Systems

In electric vehicles, reliable estimation of the state-of-charge (SoC) is crucial to determine the remaining capacity, but the electrochemical processes in metal-O2 batteries are very different to the Li-ion batteries used today, and current SoC-estimation methods prove insufficient. In Li-O2 batteries, the capacity is highly dependent on the discharge rate, since different current densities enable different growth mechanisms of Li2O2, and an on-board calibration of the SoC is therefore needed. Such a calibration is typically performed by measuring the open-circuit voltage (OCV), but as the OCV of many metal-O2 battery does not change as a function of capacity, this method cannot be used. In this manuscript, we propose a method, based on a single-frequency electrochemical impedance measurement, to estimate the remaining capacity and assess the state-of-health of reversible metal-O2 batteries by calculating the capacitance of the positive electrode where the discharge products are formed. The results from experiments on Li-O2 batteries show that the capacitance is a good measure of the remaining capacity and that the SoC estimation can be improved significantly by the calibration.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials
Authors: Christensen, A. E. (Intern), Højberg, J. (Intern), Norby, P. (Intern), Vegge, T. (Intern)
Pages: A2075-A2079
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of The Electrochemical Society
Volume: 162
Issue number: 10
ISSN (Print): 0013-4651
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 3.48 SJR 1.267 SNIP 1.009
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.97 SJR 1.222 SNIP 0.963
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.115 SNIP 1.066 CiteScore 3.17
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.213 SNIP 1.25 CiteScore 3.36
Improved Accuracy of Density Functional Theory Calculations for CO2 Reduction and Metal-Air Batteries

Density functional theory (DFT) calculations have greatly contributed to the atomic level understanding of electrochemical reactions. However, in some cases, the accuracy can be prohibitively low for a detailed understanding of, e.g. reaction mechanisms. Two cases are examined here, i.e. the electrocatalytic reduction of CO2 and metal-air batteries. In theoretical studies of electrocatalytic CO2 reduction, calculated DFT-level enthalpies of reaction for CO2 reduction to various products are significantly different from experimental values[1-3]. In theoretical studies of metal-air battery reactions, systematic errors compared to experiments have also been found in calculation of enthalpies of formation for bulk metal oxide, peroxide and superoxide species[4,5]. It is here demonstrated how the errors, which depend explicitly on the choice of applied exchange-correlation functional, can be identified through first principle methods. Ensembles generated using a Bayesian error estimation functional, in this case the BEEF-vdW functional[6], are used for the error identification. The ensembles, which consist of perturbations of the main van der Waals density functional, can be generated at low computational cost. It has previously been demonstrated how these ensembles can be used to estimate the magnitude of functional dependent errors[6]. When here applied for identification of the source of functional dependent
systematic errors, ensembles for different reactions are not only examined individually, but compared to determine patterns in functional dependence. The method is exemplified by ensemble comparison of reaction enthalpy to methanol and formic acid depicted in Figure 1. The functional dependence on the calculated reaction enthalpy to methanol is twice as large as that to formic acid. This suggests that the systematic error is due to carbon-oxygen double bonds, as the change in number of carbon-oxygen double bonds in the reaction to methanol is two as compared to one for reaction to formic acid. This is subsequently confirmed by further comparisons of functional dependence and a significant source of systematic errors in DFT-level computational electrocatalytic CO2reduction is hence identified. The new insight adds increased accuracy e.g., for reaction to formic acid, where the experimental enthalpy of reaction is 0.15 eV. Previously, this enthalpy has been calculated without and with correctional approaches to 0.39 eV and 0.30 eV, respectively[2]. Here, correcting the newly identified error in an otherwise similar approach as used previously the enthalpy of reaction is 0.13 eV. For metal-air batteries the previously observed large systematic errors are found not to be intrinsic to the metal oxide species. Errors can be significantly reduced by using metal chlorides as energy reference rather than pure metals. The mean absolute error per oxygen versus experiments for alkali metal peroxide and superoxide species will be 0.03 eV and 0.09 eV, respectively, using metal chlorides as reference, as compared to 0.47 eV and 0.17 eV using metals as reference. The presented approach for error identification is expected to be applicable to a very broad range of systems. References: [1] A. A. Peterson, F. Abild-Pedersen, F. Studt, J. Rossmeisl, and J. K. Nørskov, Energy Environ. Sci., 3,1311 (2010) [2] F. Studt, F. Abild-Pedersen, J. B. Varley, and J. K. Nørskov, Catal. Lett., 143, 71 (2013) [3] K. Chan, C. Tsai, H. A. Hansen, and J. K. Nørskov, Chem. Cat. Chem., 6, 1899 (2014) [4] J. S. Hummelshøj, A. C. Luntz, and J. K. Nørskov, J. Chem. Phys., 138, 034703 (2013) [5] S. Kang, Y. Mo, S. P. Ong, and G. Ceder, Nano Lett., 14, 1016 (2014) [6] J. Wellendorff, K. T. Lundgaard, A. Mögelhøj, V. Petzold, D. D. Landis, J. K. Nørskov, T. Bligaard, and K. W. Jacobsen, Phys. Rev. B, 85, 235149 (2012) Figure 1: Calculated enthalpies of reaction from CO2 to CH3OH (x axis) and HCOOH (y axis). Functional variations between the two are seen to correlate with slope 0.5 consistent with a systematic error on carbon-oxygen double bonds. [Figure]
Influence of Functionality on Direct Arylation of Model Systems as a Route Toward Fluorinated Copolymers via Direct Arylation Polymerization (DArP)

A screening of direct arylation conditions on a model small molecule system is carried out to develop suitable conditions for the direct arylation polymerization (DArP) of fluorinated copolymers, which are incompatible with conditions previously utilized successfully for nonfluorinated systems. The model system features a coupling between a 2-substituted
thiophene and a pentafluorobenzene, where one of the partners was brominated. A substantial difference in reactivity is observed, demonstrating that the optimal functionalization for direct arylation between a thiophene-based donor and a highly fluorinated acceptor is a halogenated thiophene and an unfunctionalized fluorinated unit, which is opposite of typical cross coupling reactions, where the acceptor is typically halogenated. The best conditions are applied to the copolymerization of 1,2,4,5-tetrafluorobenzene and 2,2’-(2,5-bis((2-hexyldecyl)oxy)1,4-phenylene)dithiophene. Polymers are free of β-defects and significant homocoupling. This work further underscores the attractive simplicity, relevance, and ease of DArP while reconfirming its broad compatibility with increasingly popular fluorinated copolymers.

**General information**

State: Published
Organisations: Department of Energy Conversion and Storage, Functional organic materials, University of Southern California
Authors: Livi, F. (Intern), Gobalasingham, N. S. (Ekstern), Bundgaard, E. (Intern), Thompson, B. C. (Ekstern)
Number of pages: 8
Pages: 2598-2605
Publication date: 2015
Main Research Area: Technical/natural sciences

**Publication information**

Journal: Journal of Polymer Science. Part A, Polymer Chemistry
Volume: 53
ISSN (Print): 0887-624X
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 0.673 SJR 0.735 CiteScore 2.45
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.83 SJR 1.069 SNIP 0.782
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.002 SNIP 0.854 CiteScore 2.93
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.101 SNIP 0.95 CiteScore 3.05
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.165 SNIP 0.996 CiteScore 3.41
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.5 SNIP 0.99 CiteScore 3.33
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.653 SNIP 0.998 CiteScore 3.64
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.761 SNIP 1.038
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 2.247 SNIP 1.111
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.936 SNIP 1.131
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 2.067 SNIP 1.159
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.96 SNIP 1.274
Influence of hydroxyl content of binders on rheological properties of cerium-gadolinium oxide (CGO) screen printing inks

The influence of hydroxyl content of binders on rheological properties of screen printing inks is investigated. The actual amount of hydroxyl groups is correlated to the level of hyper-entanglement that characterizes the binders in solution. Three of the most used binders (ethyl cellulose, and two vinyl resins) were selected and characterized in solution via viscosimetry method. A high degree of hyper-entanglement was observed for ethyl cellulose polymers, whereas a mitigated effect characterized the two vinyl resins. Cerium-gadolinium oxides (CGO)-based inks, prepared using the selected binders, were investigated by means of rheology. The vinyl resin at higher hydroxyl content and low level of hyper-entanglement was demonstrated to impart superior printability properties.

General information

State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Applied Electrochemistry, Mixed Conductors, Topsoe Fuel Cell
Number of pages: 10
Pages: 1495–1504
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information

Journal: Journal of the European Ceramic Society
Volume: 35
Issue number: 5
ISSN (Print): 0955-2219
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 3.55 SJR 1.068 SNIP 1.698
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.25 SJR 1.142 SNIP 1.888
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.135 SNIP 1.817 CiteScore 3.03
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.163 SNIP 2.083 CiteScore 3.16
Web of Science (2014): Indexed yes
Influence of interface reactions on the YBCO films grown by fluorine-free solution route

Fabrication of full-stacked coated conductors by all-chemical-solution routes exhibit a great potential in view of further reducing the cost and increasing the throughput for industrialization. Growth of YBa2Cu3O7−x (YBCO) superconducting films by fluorine-free metal organic deposition routes (FF-MOD) which are environmental friendly has attracted more attentions recently. In this work, comparison study was performed on the YBCO-Ag superconducting thin films deposited on two types of single crystal substrates, LaAlO3 and Ce0.9La0.9O2−y/YSZ. The structural characterization and superconducting properties studies reveal that the interface reactions between the YBCO-Ag film and the CLO cap layer play an essential role on the nucleation and growth of YBCO-Ag films from the FF solution. Weak texture caused by serious interface reactions at high growth temperature is the main explanations for the poor superconducting performance when using CLO/YSZ as substrate. Further investigation of compatibility of the buffer layer for FF-derived YBCO films is needed.
Influence of manganite powder grain size and Ag-particle coating on the magnetocaloric effect and the active magnetic regenerator performance

The magnetocaloric performance of $\text{La}_{0.67}\text{Ca}_{0.27}\text{Sr}_{0.06}\text{Mn}_{1.05}\text{O}_3$ is investigated as a function of the powder grain size and also as a function of decoration of grains with highly conductive silver particulates as a coating layer. We demonstrate that the thermal and electrical conductivities can be significantly modified by the Ag-particle coating when the material is examined in sintered pellet form and we compare results with a second manganite composition $\text{La}_{0.67}\text{Ca}_{0.33}\text{MnO}_3$ with significantly smaller grain size. However, we find that this microstructural engineering does not improve the performance of the active magnetic regenerator cycle using the silver decorated material in powder form. The regenerator performance is improved by the reduction of the powder grain size of the refrigerant which we attribute to improved thermal management due to increased surface to volume ratio. © 2015 Acta Materialia Inc. Published by Elsevier Ltd. All rights reserved.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Imperial College London
Authors: Turcaud, J. (Ekstern), Neves Bez, H. (Intern), Ruiz-Trejo, E. (Ekstern), Bahl, C. (Intern), Nielsen, K. K. (Intern), Smith, A. (Intern), Cohen, L. (Ekstern)
Pages: 413–418
Publication date: 2015
Main Research Area: Technical/natural sciences
Publication information
Journal: Acta Materialia
Volume: 97
ISSN (Print): 1359-6454
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 6.18 SJR 3.263 SNIP 2.737
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 5.67 SJR 3.21 SNIP 2.702
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 3.417 SNIP 2.831 CiteScore 5.22
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 3.885 SNIP 3.166 CiteScore 5.16
Web of Science (2014): Indexed yes
Influence of Side Chain Position on the Electrical Properties of Organic Solar Cells Based on Dithienylbenzothiadiazole-alt-phenylene Conjugated Polymers

Seven conjugated copolymers, based on dithienylbenzothiadiazole and benzene, have been synthesized with side chains placed in different position along the conjugated backbone. An additional polymer with a small modification of the investigated backbone was also included in the study. Alkoxy and alkyl side chains were considered, depending on the aromatic ring they were anchored to. Our goal was to perform an extensive study, by evaluating the possible anchoring positions of the same backbone, in order to demonstrate the huge influence of the position of side chains on a well performing polymer backbone for polymer solar cells. All the polymers were roll slot die coated under ambient conditions on flexible ITO-free plastic substrates to give inverted polymer solar cell devices with an upscaled active area of 1 cm². The best characteristics were found for the polymer carrying alkoxy side chains on the benzene ring where power conversion efficiencies of up to 3.6% were achieved. All studied materials were prepared with an objective of low-cost starting materials, simple synthesis, and simple processing conditions which was most successful for the polymer P5. The
polymer P7 containing fluorine atoms showed excellent performance under constant illumination and high temperature (exhibiting stable photovoltaic properties even after 670 h under conditions similar to ISOS-L-2 lifetime protocol). This makes P7 a good candidate for further upscaling and device optimization. The photovoltaic performance results were corroborated with full optical and morphological characterization of the conjugated polymers. We conclude that the determination of the best anchoring position for the side chains is the most rational starting point for the optimization of a polymer with a potential for large-scale fabrication of polymer solar cells.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Functional organic materials
Pages: 3481–3492
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Macromolecules
Volume: 48
Issue number: 11
ISSN (Print): 0024-9297
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): SJR 2.419 SNIP 1.513 CiteScore 5.86
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 5.76 SJR 2.564 SNIP 1.483
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 2.357 SNIP 1.599 CiteScore 5.82
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.524 SNIP 1.695 CiteScore 5.83
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.578 SNIP 1.736 CiteScore 6.09
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 2.78 SNIP 1.568 CiteScore 5.35
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 2.556 SNIP 1.571 CiteScore 5.15
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 2.516 SNIP 1.496
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.971 SNIP 1.512
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 2.834 SNIP 1.522
Web of Science (2008): Indexed yes
Influence of SrF$_2$ on the Formation, Microstructure and Critical Temperature of (Bi,Pb)$_{2}$Sr$_2$Ca$_2$Cu$_3$O$_{10}$ Polycrystalline Samples

Bulk ceramic samples with Bi$_{1.72}$Pb$_{0.34}$Sr$_{1.87}$Ca$_{1.91}$Cu$_{3.13}$O$_{9.83-x}$ F$_{2x}$ (0.00 ≤ x ≤ 0.51) nominal compositions were synthesized by a solid-state route using SrF$_2$ as a fluorine source. Notwithstanding of the stage, at which SrF$_2$ was introduced into the precursor powders (prior to or after calcination), a significant lowering of the reaction temperature was observed. For a fixed sintering temperature, SrF$_2$ results in an enhanced grain growth. However, the lattice parameters of the Bi$_{2223}$ phase and its superconducting transition temperature are not significantly affected by the presence of fluorine. The beneficial effect of SrF$_2$ in terms of promoted Bi$_{2223}$ phase formation appears to be limited to low SrF$_2$ contents. It is believed that the observed effects are due to the fact that an increasing proportion of Sr is kept apart from the reaction for increasing SrF$_2$ level, rather than to a direct involvement of fluorine.
Lithium ion battery technology is the heart in operating modern technology devices such as mobile phones and laptops. However, as our society is moving towards the utilization of sustainable energy sources, batteries can be foreseen to become an even more important part of the energy infrastructure. They will be used not only for transportation, but also for medium and short term storage as well as for frequency stabilization in intermittent grid scale energy sources such as solar and wind. Thus, the development of new cheaper and safer battery materials with high energy and power density is very important for a successful worldwide energy transition. The understanding of structural and compositional changes of bulk electrodes in batteries is undoubtedly important. However, it is often transport of electrons and ions across and through interfaces [1] (e.g., between lithiated and delithiated domains) which limits the obtainable power density and battery life time. A challenging and important task is to obtain in situ information about the formation and evolution of interfaces in an operating battery system. This work addresses these challenges and for this purpose we have developed a special microcapillary battery cell allowing diffraction information to be obtained from only the active material during battery operation [2]. High resolution synchrotron x-ray powder diffraction technique has been undertaken to obtain detailed structural and compositional information during lithiation/delithiation of commercial LiFePO4 materials [3]. We report results from the first in situ time resolved high resolution powder diffraction experiments at beamline ID22/31 at the European Synchrotron Radiation Facility, ESRF. We follow the structural changes during charge of commercial LiFePO4 based battery materials using the Rietveld method. Conscientious Rietveld analysis shows slight but continuous deviation...

**In Situ Studies of Fe^{4+} Stability in β-Li3Fe2(PO4)3 Cathodes for Li Ion Batteries**

In commercial Fe-based batteries the Fe^{2+}/Fe^{3+} oxidation states are used, however by also utilizing the Fe^{4+} oxidation state, intercalation of up to two Li ions per Fe ion could be possible. In this study, we investigate whether Fe^{4+} can be formed and stabilized in β-Li3Fe2(PO4)3. The work includes in situ synchrotron X-ray powder diffraction studies (XRPD) during charging of β-Li3Fe2(PO4)3 up to 5.0 V vs. Li/Li+. A novel capillary-based micro battery cell for in situ XRPD has been designed for this. During charge, a plateau at 4.5 V was found and a small contraction in volume was observed, indicating some Li ion extraction. The volume change of the rhombohedral unit cell is anisotropic, with a decrease in the a parameter and an increase in the c parameter during the Li ion extraction. Unfortunately, no increased discharge capacity was observed and Mössbauer spectroscopy showed no evidence of Fe^{4+} formation. Oxidation of the organic electrolyte is inevitable at 4.5 V but this alone cannot explain the volume change. Instead, a reversible oxygen redox process (O^{2-} → O^{−}) could possibly explain and charge compensate for the reversible extraction of lithium ions from β-Li3Fe2(PO4)3.
Scopus rating (2016): CiteScore 2.97 SJR 1.222 SNIP 0.963
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.115 SNIP 1.066 CiteScore 3.17
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.213 SNIP 1.25 CiteScore 3.36
Web of Science (2014): Indexed yes
Scopus rating (2013): SJR 1.169 SNIP 1.309 CiteScore 2.92
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.329 SNIP 1.281 CiteScore 2.61
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.331 SNIP 1.335 CiteScore 2.74
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.418 SNIP 1.304
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.442 SNIP 1.27
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.595 SNIP 1.41
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.569 SNIP 1.322
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.608 SNIP 1.535
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.523 SNIP 1.481
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.712 SNIP 1.7
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.971 SNIP 1.677
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 2.036 SNIP 1.618
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 1.663 SNIP 1.729
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 1.632 SNIP 1.7
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 1.6 SNIP 1.846

Original language: English
Batteries and Energy Storage, A
DOIs:
10.1149/2.0141504jes

Bibliographical note
Erratum in Electrochemical Society. Journal, 2015, 162(6) p. X11: Throughout this paper, the prefix “β-” has been used incorrectly to indicate the rhombohedral phase of Li3Fe2(PO4)3. The material studied in the paper is exclusively the rhombohedral phase and all instances of “β-Li3Fe2(PO4)3” should be replaced with “Li3Fe2(PO4)3.”
In Situ Synchrotron X-Ray Diffraction Characterization of the Synthesis of Graphene Oxide and Reduced Graphene Oxide

Graphene oxide (GO) and reduced graphene oxide (rGO) synthesised from GO, has a promising future in fields ranging from electronics to energy technologies[1]. GO may be synthesized by the modified Hummer’s method[2], where a mixture of potassium permanganate and concentrated sulfuric acid forms the ground pillar for the oxidation of graphite to GO. rGO can be synthesized by a broad range of methods, with the chemical and the thermal reduction routes being very common[3]. The mechanism of motion of GO by the modified Hummer’s method is still unknown, even though the active oxidizing species dimanganese heptoxide has been suggested as the main redox active specie[4]. The mechanism of the thermal reduction of GO to rGO is also unknown. We present results from in situ synchrotron X-ray diffraction (XRD) experiments of syntheses and thermal reduction of GO. The in situ synthesis of GO was performed by placing a mixture of permanganate and sulphuric acid in a capillary next to graphite. The synthesis was then initiated by gently pushing the fluid mixture into the powder with N2 gas. The in situ XRD of the GO synthesis showed how the oxidation reaction proceeds in three separate stages, as seen in Figure 1. The first stage was the dissolution of potassium permanganate, followed by an intercalation stage and subsequent formation of crystalline material. The GO 001 diffraction peak was observed early during the synthesis, in the second stage, and the intensity of the 001 diffraction increased during the third stage. The in situ XRD results of the thermal reduction of GO to rGO showed a dependence on the temperature ramping and addition of diamond powder. Syntheses were measured at 1, 5, 10, 20 and 50 °C/min temperature rams. The syntheses were performed in a capillary with GO being heated by a hot air blower under constant N2 flow. Three stages were observed for the reduction process; a GO stage, an amorphous stage and a rGO stage. The change in stage was defined from the changing of the d-value of the initial 001 GO peak, see Figure 2. The initial GO diffraction pattern changed during the heating and more diffraction peaks were observed. The results showed that the nature of the rGO material depends heavily on both temperature and additives. These in situ XRD studies revealed the crystalline intermediates and final product of synthesis by a modified Hummer’s method and the diffractional change during the thermal reduction of GO. The stages observed for both syntheses illuminate how important it is to consider the experimental parameters dependent on the application; they might even have to be optimized separately. As the future use of GO and rGO is expanding and the commercialization of these products are enhanced, the syntheses mechanisms may be of increasing interest. [1] M. Segal, Nat Nano, 4 (2009) 612-614. [2] Hummer and Offeman, J. Am. Chem. Soc. (1958) 1339-1339 [3] Pei and Cheng, Carbon (2012) 3210-3228 [4] Dreyer, Park, Bielawski and Ruoff, Chem. Soc. Rev. (2010) 228-240 [Figure]

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials
Authors: Storm, M. M. (Intern), Johnsen, R. E. (Intern), Norby, P. (Intern)
Number of pages: 1
Pages: 606
Publication date: 2015
Conference: The 228th ECS Meeting, Phoenix, Arizona, United States, 11/10/2015 - 11/10/2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Electrochemical Society. Meeting Abstracts (Online)
Volume: MA2015-02
ISSN (Print): 2151-2043
Original language: English
Source: FindIt
Source-ID: 276170139
Publication: Research - peer-review › Conference abstract in journal – Annual report year: 2015

In Situ X-Ray Diffraction Studies on Structural Changes of a P2 Layered Material during Electrochemical Desodiation/Sodiation

Sodium layered oxides with mixed transition metals have received significant attention as positive electrode candidates for sodium-ion batteries because of their high reversible capacity. The phase transformations of layered compounds during electrochemical reactions are a pivotal feature for understanding the relationship between layered structures and electrochemical properties. A combination of in situ diffraction and ex situ X-ray absorption spectroscopy reveals the phase transition mechanism for the ternary transition metal system (Fe–Mn–Co) with P2 stacking. In situ synchrotron X-ray diffraction using a capillary-based microbattery cell shows a structural change from P2 to O2 in P2–Na0.7Fe0.4Mn0.4Co0.2O2 at the voltage plateau above 4.1 V on desodiation. The P2 structure is restored upon subsequent sodiation. The lattice parameter c in the O2 structure decreases significantly, resulting in a volumetric contraction of the lattice toward a fully charged state. Observations on the redox behavior of each transition metal in P2–Na0.7Fe0.4Mn0.4Co0.2O2 using X-ray absorption spectroscopy indicate that all transition metals are involved in the reduction/oxidation process.
Instability of Ionic Liquid-Based Electrolytes in Li−O₂ Batteries

Ionic liquids (ILs) have been proposed as promising solvents for Li−air battery electrolytes. Here, several ILs have been investigated using differential electrochemical mass spectrometry (DEMS) to investigate the electrochemical stability in a Li−O₂ system, by means of quantitative determination of the rechargeability (OER/ORR), and thereby the Coulombic
efficiency of discharge and charge. None of the IL-based electrolytes are found to behave as needed for a functional Li–O2 battery but perform better than commonly used organic solvents. Also the extent of rechargeability/reversibility has been found to be strongly dependent on the choice of IL cation and anion as well as various impurities.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, Fundamental Electrochemistry, Chalmers University of Technology
Number of pages: 7
Pages: 18084–18090
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: The Journal of Physical Chemistry Part C
Volume: 119
Issue number: 32
ISSN (Print): 1932-7447
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 4.58 SJR 2.135 SNIP 1.147
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.48 SJR 1.964 SNIP 1.195
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.886 SNIP 1.26 CiteScore 4.68
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.032 SNIP 1.447 CiteScore 5.08
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 2.143 SNIP 1.445 CiteScore 5.14
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.529 SNIP 1.461 CiteScore 4.98
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.339 SNIP 1.465 CiteScore 4.92
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 2.462 SNIP 1.362
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 2.158 SNIP 1.427
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.883 SNIP 1.04
Web of Science (2008): Indexed yes
Web of Science (2007): Indexed yes
Instability of supercritical porosity in highly doped ceria under reduced oxygen partial pressure

The thermomechanical behavior and microstructural evolution of low relative density (∼0.40) gadolinium-doped ceria are characterized under oxidative and reducing conditions at high temperatures. The electronic defects generated in the structure by Ce4+ to Ce3+ reduction play an important role on all mass diffusion phenomena, including densification and grain growth. Thermodynamically stable porosity (supercritical porosity) is dominant for isothermal sintering treatments in air. Conversely, the facilitated diffusion of ions through the lattice in reducing conditions results in a nearly full densification.

© 2014 Acta Materialia Inc. Published by Elsevier Ltd. All rights reserved.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Mixed Conductors
Authors: Teocoli, F. (Intern), Ni, D. W. (Intern), Esposito, V. (Intern)
Pages: 13-16
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Scripta Materialia
Volume: 94
ISSN (Print): 1359-6462
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 4.19 SJR 1.923 SNIP 1.855
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.71 SJR 1.884 SNIP 1.737
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 2.259 SNIP 1.841 CiteScore 3.54
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.65 SNIP 2.035 CiteScore 3.55
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.323 SNIP 1.946 CiteScore 3.19
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 2.292 SNIP 1.996 CiteScore 3.01
ISI indexed (2012): ISI indexed yes
Integration of CO₂ air capture and solid oxide electrolysis for methane production

This work studied the production of substitute natural gas (SNG) from CO₂ captured from the atmosphere followed by co-electrolysis with H₂O in solid oxide electrolyzer cells (SOEC) and downstream catalytic methane production. Over the coming 20 years, Denmark is on a track to remove fossil fuels from all sectors of the energy system except for transportation. In the recently published Energikoncept 2035 [1], the Danish grid operator, Energinet.dk lays out a scenario based on 72 % wind power and 21 % biomass and waste in the electricity grid mix. In this scenario, biogas and electrolysis gasses are projected to be used for production of process heat, peak-load power generation and on the longer term to replace hydrocarbons in the most energy intensive parts of the transportation sector; especially aviation. As a prerequisite for the scenario, no biomass can be imported to enhance the supply of combustible resources. In such an energy system, technologies for production of CO₂ neutral hydrocarbons for easy storage and use in the existing infrastructure; especially in the natural gas grid; may be of great value. The studied technology fulfills those demands. The main goal of the work was to design a plant and develop a thermodynamic model of the plant operation, enabling analyses related to selection of operating parameters; analysis and optimization of internal heat recovery and integration between the main technological subsystems. Finally to identify the main areas of technological development through economic analyses. The work included experimental work on an example of a system for capture of CO₂: the humidity swing (HS) system, qualitatively evaluating the H₂O uptake and CO₂ desorption characteristics of the sorbent material, especially in relation to the supply of H₂O to the sorbent. It was found that H₂O supplied in the gas phase resulted in slow uptakes and desorption rates of CO₂ whereas supplying liquid water to the sorbent resulted in fast desorption in the first hours, after which the rate dropped sharply. A method was developed and used to characterize the impurities present in CO₂ stream from the HS system in addition to the temperature vacuum swing (TVS) system under development by Climeworks Ltd. The method relied on...
adsorption of impurities on a filter consisting of nickel-yttria-stabilised-zirconia (Ni/YSZ), similar to the material used in the fuel electrodes of SOECs followed by elemental analysis by glow discharge mass spectrometry. The method had a sub-ppm detection limit. Across the tested systems, a range of elements known to be detrimental to solid oxide cell (SOC) operation were detected in the range from tens of ppb to 20 ppm. The SNG plant was modelled using the process integration software package PRO/II alongside the design process, and a series of minor studies using PRO/II and thermodynamic analysis software FactSage® aided the design process. This included studying a long range of questions such as alternative strategies for CO₂ compression; the structure of the methanation plant; and the risk of carbon formation in both SOEC and methanation reactors, etc. The model was based on a thermodynamic 0-dimensional model of the electrolyzer sub-system, developed to technological specifications from the thermodynamic SOEC model published by Sun et al. [2] This model was used for a study of operating parameters, and two design cases were identified for the full plant based on these results. The two cases both operated at 80 atm, and had SOEC operating temperatures of 850 °C and 600 °C. The area specific resistance (ASR) of the SOECs were extrapolated to high pressure and low temperatures based on data for standard DTU Energy Ni-YSZ based cells, and the pressure dependency of the individual cell processes. With the full plant model finished, the potential for internal recovery of surplus heat was analyzed, and a network of heat exchangers synthesized in order to minimize the requirements for external heating and cooling services. Based on the process flow sheets and the heat exchanger network, the dimensions and costs of the equipment of the plant were calculated and additional cost components such as installation of equipment, land use, labor costs, operation and maintenance, etc. were estimated according to standard methods. The plant had a yearly production capacity of 575,000Nm³ of SNG with a methane content above 98.5 % which resulted in a Wobbe index of 49 MJ/Nm³ which is sufficient for injection into the natural gas grid. The SOEC stack power was around 700 kW, and the plant operated a ten energy efficiency of 65 % (HHV) and 58 % (LHV). An economic analysis based on guidelines from the Danish energy agency and standard methods was conducted accounting for interest rates, taxes, depreciation etc. at a minimum acceptable rate of return set to the minimum of 4 %. The economic analysis resulted in SNG production prices of 1.88 €/Nm³ and 2.94 €/Nm³ based on an electricity price of 18.6 €/MJ, a price of process heat at 120 °C of 11.9 €/MJ and a price of cell area of 0.23 €/cm². The main cost drivers were identified as the capital costs of the SOEC and air capture systems and the heat exchanger network. For operating costs, the electricity price had a significant impact, whereas the dependency of the SNG price on the heat price was minor. The technical issues where discussed in separate chapters interspersed by chapters documenting the modelling and design process. Finally, a comprehensive discussion at the end treats the technical issues of the plant in the light of the economic analysis.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Fundamental Electrochemistry, Applied Electrochemistry, Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry
Authors: Ebbehøj, S. L. (Intern), Mogensen, M. B. (Intern), Jensen, S. H. (Intern), Riisager, A. (Intern)
Number of pages: 263
Publication date: 2015

Publication information
Place of publication: Roskilde
Publisher: Department of Energy Conversion and Storage, Technical University of Denmark
ISBN (Print): 978-87-92986-32-0
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
Integration_of_CO2_air_capture_and_solid_oxide_electrolysis_for_methane_production.pdf

Relations
Projects:
Integration of CO₂ air capture and solid oxide electrolysis for methane production
Publication: Research › Ph.D. thesis – Annual report year: 2016

Integration of oxygen membranes for oxygen production in cement plants
The present paper describes the integration of oxygen membranes in cement plants both from an energy, exergy and economic point of view. Different configurations for oxygen enrichment of the tertiary air for combustion in the pre-calculator and full oxy-fuel combustion in both pre-calculator and kiln are examined. The economic figures of merit are compared with those from a standard cryogenic plant. Both oxygen enriched air and full oxy-fuel cases allow for an increase in clinker production, use of alternative fuels as well as on-site electricity production. In addition, the full oxy-fuel cases generate a concentrated CO2 source that can be used for enhanced oil recovery, in combination with biomass gasification and electrolysis for synthesis gas production, or possibly sequestered. The cases with oxygen enriched air provide very promising economic figures of merit with discounted payback periods slightly higher than one year. The full oxy-fuel cases have a discounted payback period of approximately 2.3 years assuming a CO2 selling price of 35 US$/ton. The sensitivity analysis of full oxy-fuel cases clearly shows that for the discounted payback period, the most sensitive parameters are the CO2 price and the clinker selling price.
Interfacial engineering of self-assembled monolayer modified semi-roll-to-roll planar heterojunction perovskite solar cells on flexible substrates

The morphologies of the perovskite (e.g. CH₃NH₃PbI₃) layer are demonstrated to be critically important for highly efficient perovskite solar cells. This work applies 3-aminopropanoic acid as a self-assembled monolayer (C₃-SAM) on a poly(3,4-ethylenedioxythiophene):poly(styrenesulfonate) (PEDOT:PSS) hole transport layer (HTL) to modify the crystallinity and coverage of the CH₃NH₃PbI₃ Cl-x(x) film, resulting in a much smoother perovskite surface morphology together with a PCE increase from 9.7% to 11.6%. Since all fabrication steps of these inverted structure devices are carried out under low temperature conditions (processing temperature <120 degrees C), it is possible to employ this method on flexible polymer substrates using roll-coating for the layer deposition. The roll-coated perovskite film on C₃-SAM modified PEDOT:PSS presents a similar trend of improvement and results in enhanced PCE from 3.7% to 5.1%. The successful application of the facile HTL modification indicates a common strategy for SAM material design and selection for efficiency enhancement in perovskite photovoltaic devices.
Investigation of Impedance-Based Parameters in Metal-O2 Batteries for Next Generation of Battery Management Systems

The need for increasing driving range in electric vehicles (EV) has led to research in high capacity batteries beyond Li-ion. Metal-O2 batteries, like Li-O2 and Na-O2, have high theoretical energy densities and thus a possibility to increase the capacity of automotive batteries significantly compared to current Li-ion batteries. A battery management system (BMS) typically uses a combination of coulomb counting and calibration based on open circuit voltage (OCV) measurements that depend on the state of charge (SOC). Calibration is needed due to the accumulation of errors in the coulomb counting. Common for most metal-O2 batteries is that the chemistry is unchanged during discharge and charge (assuming no degradation). This means that the OCV does not change as function of SOC. Furthermore, constant current measurements show a flat discharge plateau in large parts of the discharge period. This has been shown for Li-O2 and Na-O2 batteries, and in some cases also for Mg-O2 and Al-O2 batteries. Taking the well studied Li-O2 battery as an example, the dominating process during discharge is reduction of oxygen to produce Li2O2 on top of an existing Li2O2 layer. As this process continues during the entire discharge, both OCV and discharge potential is constant until the end of discharge, where other processes become limiting, as shown in figure 1. New methods have to be developed to overcome the constant OCV and flat discharge plateau that otherwise would complicate both battery management and accurate online prediction of available capacity in metal-O2 batteries. Furthermore, the increased capacity predicted for the metal-O2 batteries will result in longer discharge periods without charging, thus increasing the need for accurate calibration of the capacity in the range between ~10% and ~90% SOC. In the following we propose a method to accurately predict the capacity of metal-O2 batteries using impedance spectroscopy for calibration of the SOC tracking algorithm as well as gauging the degradation of the battery materials. This method can easily be implemented in an automotive BMS with only a few extra components and preliminary experiments have shown that the impedance measurements can be performed both during rest periods and under load conditions. This makes the method applicable not only for EVs but for batteries in a large range of electrical devices as the measurements can be performed when needed, thus maintaining a high level of accuracy for the SOC estimation and state of degradation. [1] Christensen, J., Albertus, P., Sánchez-Carrera, R. S., Lohmann, T., Kozinsky, B., Liedtke, R., et al. (2012). A Critical Review of Li/Air Batteries. Journal of the Electrochemical Society, 159(2), R1. doi:10.1149/2.086202jes [2] Hartmann, P. (2012). A rechargeable room-temperature sodium superoxide (NaO2) battery. Nature Materials, 12(3), 228–232. doi:10.1038/nmat3486 [3] Ng, K. S., Moo, C.-S., Chen, Y.-P., & Hsieh, Y.-C. (2009). Enhanced coulomb counting method for estimating state-of-charge and state-of-health of lithium-ion batteries. Applied Energy, 86(9), 1506–1511. doi:10.1016/j.apenergy.2008.11.021 [4] McCloskey, B. D., Garcia, J. M., & Luntz, A. C. (2014). Chemical and Electrochemical Differences in Nonaqueous Li–O2 and Na–O2 Batteries. The Journal of Physical Chemistry Letters, 5(7), 1230–1235. doi:10.1021/jz500494s [5] Shiga, T., Hase, Y., Kato, Y., Inoue, M., & Takechi, K. (2013). A rechargeable non-aqueous Mg–O2 battery. Chemical Communications, 49(80), 9152–9154. doi:10.1039/c3cc43477j [6] Revel, R., Audichon, T., & Gonzalez, S. (2014). Non-aqueous aluminium-air battery based on ionic liquid electrolyte. Journal of Power Sources, 272(c), 415–421. doi:10.1016/j.jpowsour.2014.08.056 [Figure]

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials
Authors: Christensen, A. E. (Intern), Højberg, J. (Intern)
Number of pages: 1
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Electrochemical Society. Meeting Abstracts (Online)
Volume: MA2015-01
Issue number: 2
Article number: 370
ISSN (Print): 2151-2043
Original language: English
Li-Air (O2) Battery I - May 26 2015 2:00PM
Links:
http://ma.ecsdl.org/content/MA2015-01/2/370.abstract?sid=92922842-3ca8-4969-ab8c-4364aee25798
Source: FindIt
Source-ID: 274862643
Publication: Research - peer-review » Conference abstract in journal – Annual report year: 2015
Investigation of Novel Electrocatalysts for Metal Supported Solid Oxide Fuel Cells - Ru:GDC

The electrochemical performance and stability of the planar metal supported solid oxide fuel cells (MS-SOFC) with two different electrocatalytically active materials, namely, Ni:GDC and Ru:GDC was investigated. Ru:GDC with an ASR of 0.322 $\Omega$cm² performed better compared to Ni:GDC with an ASR of 0.453 $\Omega$cm² at 650°C. The performance of the Ru:GDC infiltrated MS-SOFC is the best measured so far on planar MS-SOFCs. It was observed that the stability of both the electrocatalytically active materials is relatively poor. Microstructure of the anode functional layer appeared to be dense up on the examination. Further optimization of microstructure, electrocatalyst amount and electrocatalyst integration process can improve the long-term stability in particular and electrochemical performance in general.

© 2015 ECS - The Electrochemical Society
Investigation of Novel Electrocatalysts for Metal Supported Solid Oxide Fuel Cells - Ru:GDC

Even though solid oxide fuel cells (SOFCs) have a high potential with respect to efficiency and fuel flexibility they are not yet competitive in terms of cost and durability with conventional chemical energy conversion technologies. The potential cost reduction can be achieved through the development of metal supported SOFCs (MS-SOFCs) by using the cheaper support materials such as stainless steel. Furthermore, MS-SOFCs offer some advantages compared to conventional electrode and electrolyte supported SOFCs such as higher thermal conductivity, ductility in support, which are advantageous in tolerating the vibrations, transient loads, thermal and redox cycling [1-2]. The DTU MS-SOFC design based on ferritic stainless steel requires incorporation of electrocatalyst into the anode functional layer by infiltration methods [3]. Previously, the preferred electrocatalyst has been gadolinium doped ceria (GDC) with small amounts of Ni, which in the following is referred to as Ni:GDC. Recently, studies on Nb-doped SrTiO3 anode based all ceramic electrolyte supported SOFCs have shown that Ru:GDC electrocatalyst is relatively superior in terms of performance and durability than Ni:GDC [4]. In the present study, MS-SOFCs infiltrated with Ru:GDC electrocatalyst are investigated. The Ru:GDC precursor solution was infiltrated into the anode backbone and heat treated in air at different temperatures to remove the organic materials while preventing the corrosion of the metal particles. The morphology and microstructure of the infiltrated electrocatalyst layer was characterized using high-resolution electron microscopy. The electrochemical characterization involved polarization curves and electrochemical impedance spectroscopy (EIS) in the temperature range of 650-750°C. The polarization curve for Ru:GDC infiltrated MS-SOFC on single cell level (active area 16 cm2) is presented in Fig. 1. The fuel utilization corrected polarization resistance, Rp, of 0.322Ωcm2 was measured at 650°C in 20%H2O/H2. This is the lowest Rp reported for any MS-SOFC design to the knowledge of the authors. The durability was lower than expected and this could be due to the loss of percolation of the electrocatalyst. The relatively dense microstructure of the anode functional layer might have resulted in very thin electrocatalyst layer that could become non-percolating layer over the time at the operating temperature. Fig. 1 : Polarization curve of Ru:GDC infiltrated MS-SOFC at 650°C with 20%H2O/H2 fuel and air as oxidant. References: [1]. M.C. Tucker, J. Power Sources, 195 (2010) 4570-4582. [2]. P. Blennow. J. Hjelm, T. Klemenson, S. Ramousse, A. Kromp, A. Leonide, A. Weber, J. Power Sources, 196 (2011) 7117-7125. [3] T. Klemenson, J. Nielsen, P. Blennow, A.H. Persson, T. Stegk, B.H. Christensen, S. Sonderby, J. Power Sources, 196 (2011) 9459-9466. [4] T. Ramos, S. Veitze, B. R. Sudireddy, P.S. Jergensen, L. Theil Kuhn, P. Holtappels, Fuel Cells, 14 (2014) 1062-1065. [Figure]

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Applied Electrochemistry, Imaging and Structural Analysis, Mixed Conductors
Authors: Sudireddy, B. R. (Intern), Nielsen, J. (Intern), Thydén, K. T. S. (Intern), Persson, Å. H. (Intern), Brodersen, K. (Intern)
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Electrochemical Society. Meeting Abstracts (Online)
Volume: MA2015-03
Issue number: 1
Article number: 185
ISSN (Print): 2151-2043
Original language: English
Publication: Research - peer-review › Conference abstract in journal – Annual report year: 2015

Investigation of Novel Electrocatalysts for Metal Supported Solid Oxide Fuel Cells - Ru:GDC

The electrochemical performance and stability of the planar metal supported solid oxide fuel cells (MS-SOFC) with two different electrocatalytically active materials, namely, Ni:GDC and Ru:GDC were investigated. Ru:GDC with an ASR of 0.322 Ωcm2 performed better than Ni:GDC with an ASR of 0.453 Ωcm2 at 650°C. The performance of the Ru:GDC infiltrated MS-SOFC is the best measured so far on planar MS-SOFCs. It was observed that the stability of both the electrocatalytically active materials is relatively poor. Microstructure of the anode functional layer appeared to be dense up on the examination. Further optimization of microstructure, electrocatalyst amount and electrocatalyst integration process can improve the long-term stability in particular and electrochemical performance in general.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Ceramic Engineering & Science, Imaging and Structural Analysis, Mixed Conductors, Technical University of Denmark
Authors: Sudireddy, B. R. (Intern), Nielsen, J. (Ekstern), Thydén, K. T. S. (Intern), Persson, Å. H. (Intern), Brodersen, K. (Intern)
Number of pages: 10
Pages: 1417-1426
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: ECS Transactions
Volume: 68
Issue number: 1
ISSN (Print): 1938-5862
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 0.44 SJR 0.225 SNIP 0.252
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 0.4 SJR 0.228 SNIP 0.253
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.211 SNIP 0.244 CiteScore 0.36
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.212 SNIP 0.234 CiteScore 0.36
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.192 SNIP 0.231 CiteScore 0.27
ISI indexed (2013): ISI indexed no
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.241 SNIP 0.26 CiteScore 0.29
ISI indexed (2012): ISI indexed no
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.261 SNIP 0.28 CiteScore 0.36
ISI indexed (2011): ISI indexed no
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.249 SNIP 0.251
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.242 SNIP 0.27
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.254 SNIP 0.255
Scopus rating (2007): SJR 0.213 SNIP 0.206
Scopus rating (2006): SJR 0.134 SNIP 0.073
Original language: English
DOIs:
10.1149/06801.1417ecst
Publication: Research - peer-review › Conference article – Annual report year: 2016

Projects:

Lead-free piezoelectric ceramics
Department of Energy Conversion and Storage
Period: 01/08/2018 – …
Number of participants: 5
Phd Student:
Ferrero, Gianni (Intern)
Supervisor:
Dam-Johansen, Kim (Intern)
Bjørnseth Haugen, Astri (Intern)
Ringgaard, Erling (Intern)
Main Supervisor:
Sudireddy, Bhaskar Reddy (Intern)
Financing sources
Source: Internal funding (public)
Name of research programme: Industrial PhD
Project: PhD

Electrochemical CO2 reduction at high temperature in Solid Oxide Electrolysis Cells
Department of Energy Conversion and Storage
Period: 01/05/2018 → 30/04/2021
Number of participants: 3
PhD Student:
Sala, Elena Marzia (Intern)
Supervisor:
Mogensen, Mogens Bjerg (Intern)
Main Supervisor:
Chatzichristodoulou, Christodoulos (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Fonde
Project: PhD

Three-dimensional inversion of X-ray phase contrast tomography data
Department of Energy Conversion and Storage
Period: 01/05/2018 → 30/04/2021
Number of participants: 4
PhD Student:
Slyamov, Azat (Intern)
Supervisor:
Holzner, Christian (Ekstern)
Mokso, Rajmund (Ekstern)
Main Supervisor:
Andreasen, Jens Wenzel (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Marie Curie (EU-stipendium)
Project: PhD

In situ structural characterization of multilayer formation during large-scale processing of 3rd generation solar cells
Department of Energy Conversion and Storage
Period: 01/03/2018 → 28/02/2021
Number of participants: 4
PhD Student:
Sørensen, Michael Korning (Intern)
Supervisor:
Kuhn, Luise Theil (Intern)
Trofod, Thue (Intern)
Main Supervisor:
Andreasen, Jens Wenzel (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Anden EU-finansiering
Project: PhD

The Effect of Non-magnetic Properties on Active Magnetic Regeberator Performance
Department of Energy Conversion and Storage
Period: 01/03/2018 → 28/02/2021
Number of participants: 4
Phd Student:
Liang, Jierong (Intern)
Supervisor:
Engelbrecht, Kurt (Intern)
Nielsen, Kaspar Kirstein (Intern)
Main Supervisor:
Bahl, Christian (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Stipendie fra udlandet
Project: PhD

Tracking the Microstructure Evolution of an Operating Lithium-Sulphur Battery in Three Dimensions
Department of Energy Conversion and Storage
Imaging and Structural Analysis
Chalmers University of Technology
Period: 16/02/2018 → 17/08/2018
Number of participants: 2
x-ray tomography, battery
Acronym: TrackBat
Project ID: DTU-034
Number of related Ph.D. students: 0
Project Manager, academic:
Bowen, Jacob R. (Intern)
Project applicant:
De Angelis, Salvatore (Intern)

Relations
Related projects:
ESS & MAX IV: Cross border science and society

Design and Structuring of electrospun nanofiber membrane for high temperature proton exchange membrane fuel cells
Department of Energy Conversion and Storage
Period: 01/02/2018 → 31/01/2021
Number of participants: 3
Phd Student:
Chen, Yongfang (Intern)
Supervisor:
Zhang, Wenjing (Angela) (Intern)
Main Supervisor:
Li, Qingfeng (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Stipendie fra udlandet
Project: PhD

Machine Learning and AB-initio Simulations for Accelerated Materials Discovery
Department of Energy Conversion and Storage
Period: 01/02/2018 → 31/01/2021
Number of participants: 4
Phd Student:
Bölle, Felix Tim (Intern)
Supervisor:
Castelli, Ivano Eligio (Intern)
Thygesen, Kristian Sommer (Intern)
Main Supervisor:
Vegge, Tejs (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

---

**Novel electrocatalysts and 3D porous electrodes for efficient alkaline water electrolysis**
Department of Energy Conversion and Storage
Period: 01/02/2018 → 31/01/2021
Number of participants: 3
Phd Student:
Gellrich, Florian (Intern)
Supervisor:
Traulsen, Marie Lund (Intern)
Main Supervisor:
Chatzichristodoulou, Christodoulos (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Offentlig finansiering
Project: PhD

---

**Superconducting thin-film neutron detector**
Jonas Bertelsen
Department of Energy Conversion and Storage
Electrofunctional materials
Department of Wind Energy
Wind Turbine Structures and Component Design
Imaging and Structural Analysis
Period: 02/01/2018 → 20/06/2018
Number of participants: 4
Neutron detector, Superconducting thin film, Coated conductor, Thermal properties
Project participant:
Wulff, Anders Christian (Intern)
Bertelsen, Jonas Lundholm (Ekstern)
Abrahamsen, Asger Bech (Intern)
Kuhn, Luise Theil (Intern)

---

**Low-cost High Performance Thermoelectric Materials and Modules for High-temperature Waste Heat Harvesting**
The main purpose of this new network is to establish scientific collaboration between researchers at the Technical University of Denmark (DTU) with researchers from the Korea Institute of Ceramic Engineering & Technology (KICET) and National Institute for Materials Science (NIMS), Japan. This network activity is expected to enhance the core competences for both the Danish and international partners. Specific goals are: (I) to identify the major obstacles that hinder thermoelectric technology to move into the market, i.e. high performance and long-term stability of thermoelectric materials and devices under field conditions; (II) to establish a strong network between DTU, KICET, and NIMS to attract academic and industrial partners to support these activities by future funding. These goals will be supported by the visit of leading research scientists from Denmark, South Korea, and Japan in combination with participation in international conferences, seminars and a specifically organized workshop

Department of Energy Conversion and Storage
Design and structuring of electrospun nanofiber non-Pt catalysts and electrode for high temperature proton exchange membrane fuel cells

Department of Energy Conversion and Storage
Period: 01/01/2018 → 31/12/2020
Number of participants: 3
Phd Student: Bompolaki, Eftychia (Intern)
Supervisor: Zhang, Wenjing (Angela) (Intern)
Main Supervisor: Jensen, Jens Oluf (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Fonde
Project: PhD

Development of novel electrode materials for high temperature electrochemical water splitting

Department of Energy Conversion and Storage
Period: 01/01/2018 → 31/12/2020
Number of participants: 4
Phd Student: Mazzanti, Nicola (Intern)
Supervisor: Chatzichristodoulou, Christodoulos (Intern)
Mogensen, Mogens Bjerg (Intern)
Main Supervisor: Hendriksen, Peter Vang (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Fonde
Project: PhD

Getting the most out of magnetocaloric materials for high efficiency refrigeration

Department of Energy Conversion and Storage
Period: 01/01/2018 → 31/12/2020
Number of participants: 4
Phd Student: Erbesdobler, Florian (Intern)
Supervisor: Bahl, Christian (Intern)
Bjørk, Rasmus (Intern)
Main Supervisor: Nielsen, Kaspar Kirstein (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD
Mesoscale modelling of morphologies, charge carrier generation, and charge transport in third generation solar cells

Department of Energy Conversion and Storage
Period: 01/01/2018 → 31/12/2020
Number of participants: 4
Phd Student:
Gertsen, Anders Skovbo (Intern)
Supervisor:
Nelson, Jenny (Ekstern)
Stingelin-Stutzmann, Natalie (Ekstern)
Main Supervisor:
Andreasen, Jens Wenzel (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Anden EU-finansiering
Project: PhD

Organic Redox Flow Batteries: Active Materials and Cell Stability

Department of Energy Conversion and Storage
Period: 01/01/2018 → 31/12/2020
Number of participants: 3
Phd Student:
Hoffmeyer, Doris (Intern)
Supervisor:
Vegge, Tejs (Intern)
Main Supervisor:
Hjelm, Johan (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet
Project: PhD

High Resolution X-ray Diffraction Contrast Tomography

Department of Energy Conversion and Storage
Imaging and Structural Analysis
Neutrons and X-rays for Materials Physics
Period: 15/11/2017 → 14/11/2020
Number of participants: 3
Phd Student:
Lucas, Mariana Mar (Intern)
Supervisor:
Poulsen, Henning Friis (Intern)
Main Supervisor:
Andreasen, Jens Wenzel (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Anden EU-finansiering
Project: PhD

Development of a versatile slip-ring/rotary-union based in-operando high temperature functional material test cell for the DanMAX beamline

Department of Energy Conversion and Storage
Imaging and Structural Analysis
Neutrons and X-rays for Materials Physics
Period: 01/10/2017 → 31/03/2018
Number of participants: 3
X-ray synchrotron scattering
Acronym: Op-Stage
Project ID: DTU-029
Number of related Ph.D. students: 1
Project participant:
Karlsson, Maths (Ekstern)
Project Manager, academic:
Bowen, Jacob R. (Intern)
Project applicant:
Sierra Trujillo, Jose Xavier (Intern)

Relations
Related projects:
ESS & MAX IV: Cross border science and society
Project

Computational design of electrocatalysts for CO2 reduction
Department of Energy Conversion and Storage
Period: 01/09/2017 → 31/08/2020
Number of participants: 3
Phd Student:
Kildgaard, Jens Vive (Intern)
Supervisor:
Hansen, Heine Anton (Intern)
Main Supervisor:
Vegge, Tejs (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Eksternt finansieret virksomhed
Project: PhD

Development of Porous Electrodes for Alkaline Electrolyzers
Department of Energy Conversion and Storage
Period: 01/09/2017 → 31/08/2020
Number of participants: 4
Phd Student:
Reumert, Alexander Kappel (Intern)
Supervisor:
Cleemann, Lars Nilausen (Intern)
Kraglund, Mikkel Rykær (Intern)
Main Supervisor:
Jensen, Jens Oluf (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

In situ Structural Characterization of Multilayer Formation during Large-scale Processing of 3rd Generation Solar Cells
Department of Energy Conversion and Storage
Period: 01/09/2017 → 26/10/2017
Number of participants: 3
Phd Student:
Rogowska, Melania (Intern)
Supervisor:
Kuhn, Luise Theil (Intern)
**Main Supervisor:**
Andreasen, Jens Wenzel (Intern)

**Financing sources**
**Source:** Internal funding (public)
**Name of research programme:** Anden EU-finansiering
**Project:** PhD

**In-situ Ptychographic Studies of Lithium-Sulphur Micro-Batteries**
PtycoBat exploits a novel battery geometry designed to capitalize on recent gains in high-resolution imaging offered by synchrotron X-ray ptychography. This will be used to explore degradation processes in potential next generation high capacity Li-S battery technology (in-situ). It is expected that the kinetics and mechanisms of these processes will be observed for the first time and that the exploratory project will lay the groundwork for future full 3D in-situ imaging at MAXIV.

**Department of Energy Conversion and Storage**
**Imaging and Structural Analysis**

Chalmers University of Technology
**Period:** 15/08/2017 → 15/02/2018
**Number of participants:** 3
**Acronym:** PtychoBat
**Project ID:** DTU-022
**Number of related Ph.D. students:** 0
**Project participant:**
Matic, Aleksandar (Ekstern)
**Project Manager, academic:**
Bowen, Jacob R. (Intern)
**Project applicant:**
De Angelis, Salvatore (Intern)

**Relations**
**Related projects:**
ESS & MAX IV: Cross border science and society
**Project**

**3D electron microscopy of nanostructures in energy devices**

Department of Energy Conversion and Storage
**Period:** 01/08/2017 → 31/07/2020
**Number of participants:** 4
**Phd Student:**
Colding-Jørgensen, Sofie (Intern)
**Supervisor:**
Schmidt, Søren (Intern)
Simonsen, Søren Bredmose (Intern)
**Main Supervisor:**
Kuhn, Luise Theil (Intern)

**Financing sources**
**Source:** Internal funding (public)
**Name of research programme:** Institut stipendie (DTU)
**Project:** PhD

**Thermochemical Heat Storage**
Department of Energy Conversion and Storage
**Period:** 01/07/2017 → 30/06/2020
**Number of participants:** 3
**Phd Student:**
Karabanova, Anastasia (Intern)
**Supervisor:**
New Concepts for Efficient Immobilization of Enzymes in Inorganic Membrane Reactors

Department of Energy Conversion and Storage
Period: 01/06/2017 → 31/05/2020
Number of participants: 4
Phd Student:
Lehmann, Jonas (Intern)
Supervisor:
Pinelo, Manuel (Intern)
Main Supervisor:
Kaiser, Andreas (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet
Project: PhD

Nanoscale design of Ammonia Carriers for Air Pollution Control (NANOCONTROL)
Development of materials and multilayer structures for adsorption of ammonia.

Department of Energy Conversion and Storage
Ceramic Engineering & Science
Period: 01/05/2017 → 30/04/2021
Number of participants: 1
gas adsorption, ceramic processing
Acronym: NANOCONTROL
Number of related Ph.D. students: 1
Project participant:
Kaiser, Andreas (Intern)

Commercial project SOFC related

Department of Energy Conversion and Storage
Applied Electrochemistry
Period: 01/05/2017 → 30/04/2018
Number of participants: 1
Project participant:
Hagen, Anke (Intern)

Nanocrafts - proof of concept nanotechnology for jewelry industry
At DTU Nanotech several nanotechnologies were intensively used for texturing, patterning, and protection of surfaces. Nanotechnology can provide a new space for creative design in jewelry with unique features and effects (for instance optical effects implied by nanostructures), bring the deep meaning of emotions and relations to a new level – the nanolevel.
With significant value to the jewelry industry nanotechnology can result in unique technical qualities such as improved durability of items and fraud protection and data encryption technology, and a new way of sensing the item. Micro and nanopatterning allow individual design fabrication on a single wafer. With nanoceramic layers, we can protect golden or other jewelry items from mechanical damage or natural degradation. In this project, we apply
• Surface nanostructuring for physical effects enhancement
• Optical coloring with thin film deposition
• Visual patterning with laser engraving and UV photolithography
• Nanoplasmonic coloring
• Laser engraving on surfaces for data encryption and individual design patterns at the scale of few micrometers

Department of Energy Conversion and Storage

Department of Micro- and Nanotechnology

Silicon Microtechnology
Period: 01/05/2017 → 30/09/2017
Number of participants: 2
Acronym: Nanocrafts
Project participant: 
Plakhotnyuk, Maksym (Intern)
Davidsen, Rasmus Schmidt (Intern)

GIANT-E: Microstructural forging of electromechanically active bulk ceria

Department of Energy Conversion and Storage
Period: 15/04/2017 → 14/04/2020
Number of participants: 3
PhD Student: 
Kabir, Ahsanul (Intern)
Supervisor: 
Van Nong, Ngo (Intern)
Main Supervisor: 
Esposito, Vincenzo (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

SOFC stack project II

Department of Energy Conversion and Storage
Electrofunctional materials
Period: 01/04/2017 → 01/04/2018
Number of participants: 1
Project participant: 
Wulff, Anders Christian (Intern)

Fabrication and electrical properties of advanced thin film materials for resistive switching memories

Department of Energy Conversion and Storage
Period: 01/04/2017 → 31/03/2020
Number of participants: 5
PhD Student: 
Li, Yang (Intern)
Supervisor: 
Esposito, Vincenzo (Intern)
Sanna, Simone (Intern)
Traulsen, Marie Lund (Intern)
Main Supervisor: 
Pryds, Nini (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD
Synthesis and characterization of Tubular Oxygen transport membranes
Department of Energy Conversion and Storage
Period: 01/04/2017 → 31/03/2020
Number of participants: 4
PhD Student:
Martinez Aguilera, Lev (Intern)
Supervisor:
Bjørnetun Haugen, Astri (Intern)
Kaiser, Andreas (Intern)
Main Supervisor:
Kiebach, Wolff-Ragnar (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Eksternt finansieret virksomhed
Project: PhD

Giant-E - Ceria Thin Films Giant Electrostrictors
Department of Energy Conversion and Storage
Period: 15/02/2017 → 14/02/2020
Number of participants: 4
PhD Student:
Santucci, Simone (Intern)
Supervisor:
Lubomirsky, Igor (Ekstern)
Pryds, Nini (Intern)
Main Supervisor:
Esposito, Vincenzo (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Investigation of metallic-ceramic 3D network-structures for solid oxide fuel cell technology
Investigation of metallic/ceramic Cu-Mn/Cu-Mn-O spinel foam structures and development of Cu-Mn/Cu-Mn-O spinel oxide nanofibers.
Department of Energy Conversion and Storage
Electrofunctional materials
Proton conductors
Mixed Conductors
Period: 01/02/2017 → 23/06/2017
Number of participants: 4
SOFC, oxide spinnel, SEM-EDS, microstructure, thermal analysis, electrochemistry, Nanofibers, crystallography
Project participant:
Lund, Rasmus Kvist (Ekstern)
Supervisor:
Zhang, Wenjing (Angela) (Intern)
Main Supervisor:
Wulff, Anders Christian (Intern)
Project

Modelling of ultrafast scattering experiments probing electronic dynamics in solar cells
Department of Energy Conversion and Storage
Period: 15/01/2017 → 14/01/2020
Number of participants: 3
Phd Student:
Khalili, Khadijeh (Intern)
Supervisor:
Santra, Robin (Ekstern)
Main Supervisor:
Andreasen, Jens Wenzel (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Anden EU-finansiering
Project: PhD

Implementation in real SOFC Systems of monitoring and diagnostic tools using signal analysis to increase their lifetime
Department of Energy Conversion and Storage
Applied Electrochemistry
Period: 02/01/2017 → 31/12/2019
Number of participants: 1
Acronym: INSIGHT
Project ID: INSIGHT
Number of related Ph.D. students: 1
Project participant:
Hagen, Anke (Intern)
Project

Commercial project SOFC related
Department of Energy Conversion and Storage
Applied Electrochemistry
Period: 02/01/2017 → 31/03/2017
Number of participants: 1
Project participant:
Hagen, Anke (Intern)
Project

Nanofiber structures for efficient enzyme immobilization in membrane applications
International Network Project between DTU and Mahatma Gandhi University (MGU) and other partners from India
Department of Energy Conversion and Storage
Ceramic Engineering & Science
Period: 01/01/2017 → 31/12/2017
Number of participants: 1
Membranes, electrospinning, water filtration, ceramic processing, nanofibers, enzymes
Project ID: 6144-00035A
Project participant:
Kaiser, Andreas (Intern)
Project

The fabrication and testing of two terminal memristor device - Nano Ionic Conducting Engineered materials for information application
Department of Energy Conversion and Storage
Ceramic Engineering & Science
Electrofunctional materials
A novel off-grid thermoelectric-photovoltaic desalination system

Desalination of brackish water/sea water is a sustainable way to meet water demand in arid locations. A number of humidification/dehumidification (HDH) devices based on conventional vapor compression technology are currently available. However, these devices have a number of inherent problems such as high noise levels, compressor vibration and excessive weight and size.

The overall objective of the project is to develop and demonstrate a novel off-grid desalination system using thermoelectric technology combined with a photovoltaic system.

The combination of photovoltaic (PV) and thermoelectric (TE) technologies will not only overcome the problems of a conventional desalination system, but it also brings many additional advantages such as being off-grid, having less moving parts, easy to install, less maintenance, and on top being environmentally friendly.

The outcome of the project will be:
(i) High performance thermoelectric-solar desalination prototype to cheaply produce potable water with a targeted coefficient of performance (COP) of more than 1.5.
(ii) Demonstration of a future environmentally friendly energy technological concept with high commercial potential.

In this project, DTU Energy, AquaDania A/S, SunPower Applications A/S, and All Things Considered A/S work closely together toward a goal to develop a novel off-grid desalination system using a thermoelectric module coupled with a PV system. We address the needs of people's drinking water in remote areas of the world, or the emergency needs of catastrophic situation especially people living in arid countries.

Advanced tailoring of 3D microstructures for superconducting magnets

Superconducting magnets capable of producing large magnetic fields are indispensible for magnetic resonance imaging (MRI) for medical diagnostics. The higher the field is, the higher the spatial resolution achievable in the scanner is; this is crucial for the early detection of, e.g., cancer tumors. The present research project focuses on a new concept for the superconducting magnet which will enable an increase in the magnetic field by a factor of more than three. This is done by using ceramic superconductors in combination with a novel substrate configuration recently developed by the applicant. The substrate makes it possible to produce many thin superconducting 3D structured filaments instead of a single wide conductor, thus increasing the field produced and improving the resolution of the MRI device. The project aims to solve the scientific problems currently impeding the achievement of sufficiently small filaments. A major scientific problem is related
to oxygen formation and spread during electro-etching of 3D profiles resulting in undesired structural filament variations.

Department of Energy Conversion and Storage

Electrofunctional materials

Imaging and Structural Analysis
Period: 01/01/2017 → 01/01/2019
Number of participants: 7

Surface modification, electrochemistry, topography, Coated conductor, Superconductor, ceramic processing

Acronym: ATOMIS
Project ID: DFF – 6111-00252
Project participant:
Insinga, Andrea Roberto (Intern)
Grivel, Jean-Claude (Intern)
Nielsen, Pernille Hedemark (Intern)
Wichmann, Mike (Intern)
Usoskin, Alexander (Ekstern)
Gömöry, Fedor (Ekstern)

Project Manager, academic:
Wulff, Anders Christian (Intern)

Adhesive development for flexible thin film electronic encapsulation

Department of Energy Conversion and Storage
Period: 01/01/2017 → 31/12/2019
Number of participants: 3

Phd Student:
Kovrov, Aleksandr (Intern)
Supervisor:
Helgesen, Martin (Intern)
Main Supervisor:
Søndergaard, Roar R. (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Density functional theory based modelling of materials for resistive switching memories

Department of Energy Conversion and Storage
Period: 01/01/2017 → 31/12/2019
Number of participants: 4

Phd Student:
Pedersen, Christian Søndergaard (Intern)
Supervisor:
Pryds, Nini (Intern)
Vegge, Tejs (Intern)
Main Supervisor:
García Lastra, Juan Maria (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

DronEL
The purpose of this project is to develop and bring to market an aerial drone based automated solution (DronEL) used for a full PV plant survey for more accurate survey in less time. The automatic drone-based inspection method combines IR, EL and PL imaging, and visual images.
Department of Photonics Engineering
Diode Lasers and LED Systems
Coding and Visual Communication
Centre of Excellence for Silicon Photonics for Optical Communications
Department of Energy Conversion and Storage
Organic Energy Materials
Aalborg University
Sky Watch
SiCon
Kenergy
Skive Kommune
Period: 01/01/2017 → 31/12/2019
Number of participants: 8
Project ID: 71001
Project participant:
Thorsteinsson, Sune (Intern)
Forchhammer, Søren (Intern)
Benatto, Gisele Alves dos Reis (Intern)
Riedel, Nicholas (Intern)
Thorseth, Anders (Intern)
Dam-Hansen, Carsten (Intern)
Mantel, Claire (Intern)
Project Manager, organisational:
Poulsen, Peter Behrensdoeff (Intern)

Relations
Related projects:
PV LED ENGINE
PV BALCONY FENCE – a highly esthetic cost efficient PV integrated balcony
Activities:
7th International SpectroRadiometer Comparison (ISRC 2017)
Activities in the standardisation of light sources and spectroradiometer calibration
Outdoor Electroluminescence Acquisition Using a Movable Testbed
Publications:
New dental applications with LEDs
Quantification of solar cell failure signatures based on statistical analysis of electroluminescence images
Luminescence Imaging Strategies for Drone-Based PV Array Inspection
Indoor measurement of angle resolved light absorption by antireflective glass in solar panels
New Light Source Setup for Angle Resolved Light Absorption measurement of PV sample
Optimizing sensitivity of Unmanned Aerial System optical sensors for low zenith angles and cloudy conditions
Development of outdoor luminescence imaging for drone-based PV array inspection

Freeze casting to create micro-channel structures
Department of Energy Conversion and Storage
Period: 01/01/2017 → 31/12/2019
Number of participants: 3
Phd Student:
Christiansen, Cathrine Deichmann (Intern)
Supervisor:
Nielsen, Kaspar Kirstein (Intern)
Main Supervisor:
Theoretical investigations of the sudden death process in metal-air batteries

Department of Energy Conversion and Storage
Period: 01/01/2017 → 31/12/2019
Number of participants: 3
Phd Student:
Tygesen, Alexander Sougaard (Intern)
Supervisor:
Vegge, Tejs (Intern)
Main Supervisor:
García Lastra, Juan Maria (Intern)

Advanced neutron imaging of energy devices in 2D and 3D

Department of Energy Conversion and Storage
Period: 15/12/2016 → 14/12/2019
Number of participants: 5
Phd Student:
Lacatusu, Monica-Elisabeta (Intern)
Supervisor:
Johnsen, Rune E. (Intern)
Schmidt, Søren (Intern)
Strobl, Markus (Ekstern)
Main Supervisor:
Kuhn, Luise Theil (Intern)

Improving the interface adherence in solid oxide fuel cell stacks

Department of Energy Conversion and Storage
Period: 15/12/2016 → 14/12/2019
Number of participants: 4
Phd Student:
Ritucci, Ilaria (Intern)
Supervisor:
Agersted, Karsten (Ekstern)
Frandsen, Henrik Lund (Intern)
Main Supervisor:
Kiebach, Wolff-Ragnar (Intern)
Solid oxide fuel cells and biogas
Department of Energy Conversion and Storage
Period: 15/12/2016 → 14/12/2019
Number of participants: 4
Phd Student:
Langnickel, Hendrik (Intern)
Supervisor:
Graves, Christopher R. (Intern)
Olsen, Rasmus (Ekstern)
Main Supervisor:
Hagen, Anke (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Novel Anodes for Solid Oxide Fuel Cells
Department of Energy Conversion and Storage
Period: 01/11/2016 → 31/10/2019
Number of participants: 4
Phd Student:
Drasbæk, Daniel Bøgh (Intern)
Supervisor:
Sudireddy, Bhaskar Reddy (Intern)
Traulsen, Marie Lund (Intern)
Main Supervisor:
Holtappels, Peter (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Novel Cobalt Free Oxygen Electrodes for Solid Oxide Electrolysis Cells
Department of Energy Conversion and Storage
Period: 01/11/2016 → 31/10/2019
Number of participants: 4
Phd Student:
Tong, Xiaofeng (Intern)
Supervisor:
Hendriksen, Peter Vang (Intern)
Ovtar, Simona (Intern)
Main Supervisor:
Chen, Ming (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Stipendie fra udlandet
Project: PhD

Cost and energy effective all-black solar cell panel | Black Si BIPV | Phase 2
The objective of the EUDP project is to develop and manufacture a novel type of solar panel based on a new type of solar cell (black silicon solar cell), which – apart from a high and preferably improved efficiency and an implementable and cheaper production method – should have several significant advantages in terms of building integration. The black solar cells will be further processed to make the front conducting grid completely black through an electrochemical deposition technology. The tabbing wires interconnecting the cells in the panel will be processed into non-reflecting black strings in a scalable, inorganic electrochemical process step securing a completely black appearance of the solar panel later
produced. A compatible panel production process with traditional PV panel process will be demonstrated for the total black silicon BIPV module.

Department of Photonics Engineering
Diode Lasers and LED Systems
Department of Micro- and Nanotechnology
Silicon Microtechnology
Experimental Surface and Nanomaterials Physics
Department of Energy Conversion and Storage
Organic Energy Materials
Gaia Solar A/S
Institute for Product Development
SoliTek

Nines Photovoltaics
Period: 01/10/2016 → 30/09/2018
Number of participants: 7
BIPV, Black Silicon
Acronym: BS2
Project participant:
Thorsteinsson, Sune (Intern)
Davidsen, Rasmus Schmidt (Intern)
Iandolo, Beniamino (Intern)
Hansen, Ole (Intern)
Riedel, Nicholas (Intern)
Benatto, Gisele Alves dos Reis (Intern)
Project Manager, organisational:
Poulsen, Peter Behrensdruff (Intern)

Modeling of Large-Scale Electricity Storage Systems based on Pressurized Reversible Solid Oxide Cells
Master of Science Thesis
Department of Mechanical Engineering
Thermal Energy
Risø National Laboratory for Sustainable Energy
Department of Energy Conversion and Storage
Applied Electrochemistry
Period: 01/10/2016 → 28/02/2017
Number of participants: 4
Natural Gas, Electricity Storage, Natural gas grid, Pressurized Solid Oxide Cells, Highly Efficient Storage, Bio-Syngas Upgrade
Project participant:
Butera, Giacomo (Intern)
Supervisor:
Jensen, Søren Højgaard (Intern)
Campanari, Stefano (Ekstern)
Main Supervisor:
Clausen, Lasse Røngaard (Intern)
Documents:
Giacomo_Butera_Master_Thesis_2015_2016
Project
The concept will be tested by a Danish industrial player, NOLIAC, for biomedical applications.

Department of Energy Conversion and Storage
Ceramic Engineering & Science

Modeling of degradation processes in high temperature electrolysis cells

Department of Energy Conversion and Storage
Period: 01/09/2016 → 31/08/2019
Number of participants: 4
Phd Student:
Trini, Martina (Intern)
Supervisor:
Hauch, Anne (Intern)
Hendriksen, Peter Vang (Intern)
Main Supervisor:
Chen, Ming (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD
Nano-Editor: Development of nano-materials based printing media for all-ceramic solid oxide fuel cells manufacturing

Department of Energy Conversion and Storage
Period: 01/09/2016 → 31/08/2019
Number of participants: 3
Phd Student:
Rosa, Massimo (Intern)
Supervisor:
Zielke, Philipp (Intern)
Main Supervisor:
Esposito, Vincenzo (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Anden EU-finansiering
Project: PhD

X-ray phase contrast nano-tomography of 3rd generation solar cells

Department of Energy Conversion and Storage
Period: 01/09/2016 → 31/08/2019
Number of participants: 4
Phd Student:
Fevola, Giovanni (Intern)
Supervisor:
Carbone, Gerardina (Ekstern)
Dong, Yiqiu (Intern)
Main Supervisor:
Andreasen, Jens Wenzel (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Anden EU-finansiering
Project: PhD

Electrodeposition of Metallic 3D Surface-Profiles for Superconductor Tapes

Master thesis project by Suzanne Zamany Andersen. Thesis abstract: The work in this thesis is based on a recently introduced 3D surface-prole technique, i.e. the two-level undercut-prole substrate (2LUPS) concept [1]-[2], used for production of multi-lammary high-temperature coated conductor (CC) tapes. Reducing the superconductor lament width linearly reduces the alternating current hysteretic energy losses [3], and it enables manufacturing of stable high-temperature superconducting magnets [4]. A new process of tape masking and Ni-based electroplating on a Ni-W metal alloy substrate to form similar 3D surfaceproles as those achieved by the 2LUPS concept [5], which is based on two levels of plateaus connected via an undercut-prole, is investigated. The undercut-prole should be large enough to enable a shading effect during subsequent physical vapor deposition (PVD) of layers, thereby creating self-formed and physically separated superconductor lamnants on the two plateaus, while still utilizing the full width of the CC. This will theoretically increase the engineering current density compared to current lament techniques utilizing e.g. laser striation or mechanical scribing. Inspection of the metal substrate cross-section using focused ion beam milling and scanning electron microscopy (FIBSEM) reveals that an undercut-prole is achieved by using kapton tape as a mask while electroplating nickel to create the upper plateaus. The arithmetic surface roughness of the electroplated nickel layer is determined via atomic force microscopy (AFM) to be suitable for CC fabrication. To verify if the undercut-prole is sucient, an electrically insulating layer of SiO, simulating the buer layers in CCs, followed by an electrically conductive layer of Ag, simulating the superconducting layer, is deposited using PVD, and four-point probe measurements to create I/V characteristics are used to measure resistance across plateaus. The plateaus are deemed electrically insulated from each other, as the resistances from each insulating layer adds up to the total resistance through both plateaus. Accordingly, it is expected that these new electroplated 3D surface-proles will also enable lamentation of superconductors produced by PVD processes. A small caveat to these ndings, is the lack of a suitable prole for the use in CC fabrication being manufactured in this project. The adhesive in the masking tape creates bulges or protrusions in the prole, so a further study on thinner adhesive layers or a dierent masking material altogether is needed. The possibility of texture transfer from the Ni-W metal substrates to the plated Ni layer is also investigated, for the use in the cheaper rolling assisted bi-axially textured substrate (RABiTS) fabrication process. The electrodeposited Ni would during annealing at low temperatures experience an abnormal grain growth stage, thereby rendering it incapable of attaining the texture needed for RABiTS fabrication. Furthermore, the thermal grooving during annealing of the pure Ni could also become a problem for the ion beam assisted deposition (IBAD) process, as a surface roughness of <5nm is desired. The author of this thesis therefore strongly recommends investigating the possibility of plating e.g. Ni-W instead.
Department of Energy Conversion and Storage
Electrofunctional materials
Department of Physics
Experimental Surface and Nanomaterials Physics
Imaging and Structural Analysis
Period: 22/08/2016 → 12/02/2017
Number of participants: 5
electrochemistry, electroplating, metal substrates, Coated conductor, Superconductor, topography, EBSD, FIB-SEM, texture
Project participant:
Andersen, Suzanne Zamany (Intern)
Supervisor:
Jørgensen, Peter Stanley (Intern)
Nielsen, Pernille Hedemark (Intern)
Main Supervisor:
Wulff, Anders Christian (Intern)
Examiner:
Bentien, Anders (Ekstern)
Project

**Advanced structuring of adsorbents by electrospinning for gas cleaning and storage**

Department of Energy Conversion and Storage
Period: 15/08/2016 → 15/08/2017
Number of participants: 4
Phd Student:
Vinkel, Nadja Maria (Intern)
Supervisor:
Akhtar, Farid (Ekstern)
Zhang, Wenjing (Angela) (Intern)
Main Supervisor:
Kaiser, Andreas (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

**Co-electrolysis SOEC**

Department of Energy Conversion and Storage
Period: 15/08/2016 → 14/08/2019
Number of participants: 3
Phd Student:
Rao, Megha (Intern)
Supervisor:
Jensen, Søren Højgaard (Intern)
Main Supervisor:
Hagen, Anke (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Anden EU-finansiering
Project: PhD

**Computational design of catalysts for electroreduction of nitrogen into ammonia**

Department of Energy Conversion and Storage
Density Functional Theory Studies of Water Electrolysis on Ceria

Department of Energy Conversion and Storage
Period: 01/08/2016 → 31/07/2019
Number of participants: 3
Phd Student: Pan, Jaysree (Intern)
Supervisor: Hansen, Heine Anton (Intern)
Main Supervisor: Vegge, Tejs (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Eksternt finansieret virksomhed
Project: PhD

Cost-effective and flexible 3D printed SOFC stacks for commercial applications

A Solid Oxide Fuel Cell (SOFC) is a ceramic-based multilayer device that involves expensive and time-consuming multi-step manufacturing processes including tape casting, screen printing, firing, shaping and several high-temperature thermal treatments. In addition, these cells are manually assembled into stacks resulting in extra steps for joining and sealing that difficult the standardization and quality control of the final product while introducing weak parts likely to fail. Since current ceramics processing presents strong limitations in shape and extremely complex design for manufacturing (more than 100 steps), industrially fabricated SOFC cells and stacks are expensive and present low flexibility and long time to market. This is particularly relevant for the commercial segment of the stationary fuel cells market (5-400kW) that is highly heterogeneous in terms of the overall power and heat requirements and requires customization of the final product. The main goal of the Cell3Ditor project is to develop a 3D printing technology for the industrial production of SOFC stacks by covering research and innovation in all the stages of the industrial value chain (inks formulation, 3D printer development, ceramics consolidation and system integration). All-ceramic joint-free SOFC stacks with embedded fluidics and current collection will be fabricated in a two-step process (single-step printing and sintering) to reduce in energy, materials and assembly costs while simplifying the design for manufacturing and time to market. Compared to traditional ceramic processing, the Cell3Ditor manufacturing process presents a significantly shorter time to market (from years to months) and a cost reduction estimated in 63% with an initial investment below one third of an equivalent conventional manufacturing plant (production of 1000 units per year). The project is product-driven and involves SMEs (with proved technologies) in the entire value chain to ensure reaching TRL>6.

Department of Energy Conversion and Storage
Ceramic Engineering & Science
Period: 01/07/2016 → 31/12/2019
Number of participants: 2
Acronym: Cell3Ditor
Project participant: Esposito, Vincenzo (Intern)
Rosa, Massimo (Intern)

Development and pressure testing of solid oxide electrolyser cells
Breaking the temperature limits of Solid Oxide Fuel Cells: Towards a new family of ultra-thin portable power sources

Solid Oxide Fuel Cells (SOFCs) are one of the most efficient and fuel flexible power generators. However, a great limitation on their applicability arises from temperature restrictions. Operation approaching room temperature (RT) is forbidden by the limited performance of known electrolytes and cathodes while typical high temperatures (HT) avoid their implementation in portable applications where quick start ups with low energy consumption are required.

The ULTRASOFC project aims breaking these historical limits by taking advantage of the tremendous opportunities arising from novel fields in the domain of the nanoscale (nanoionics or nano photochemistry) and recent advances in the marriage between micro and nanotechnologies. From the required interdisciplinary approach, the ULTRASOFC project addresses materials challenges to (i) reduce the operation to RT and (ii) technological gaps to develop ultra-low-thermal mass structures able to reach high T with extremely low consumption and immediate start up.

A unique μSOFC technology fully integrated in ultrathin silicon will be developed to allow operation with hydrogen at room temperature and based on hydrocarbons at high temperature. Stacking these μSOFCs will bring a new family of ultrathin power sources able to provide 100 mW at RT and 5W at high T in a size of a one-cent coin. A stand-alone device fuelled with methane at HT will be fabricated in the size of a dice.

Apart from breaking the state-of-the-art of power portable generation, the ULTRASOFC project will cover the gap of knowledge existing for the migration of high T electrochemical devices to room temperature and MEMS to high T. Therefore, one should expect that ULTRASOFC will open up new horizons and opportunities for research in adjacent fields like electrochemical transducers or chemical sensors. Furthermore, new technological perspectives of integration of unconventional materials will allow exploring unknown devices and practical applications.
Active Magnetic regenerator refrigeration with rotary multi-bed technology

Department of Energy Conversion and Storage
Period: 01/04/2016 → 20/09/2016
Number of participants: 7
Phd Student:
Eriksen, Dan (Intern)
Supervisor:
Bahl, Christian (Intern)
Bjørk, Rasmus (Intern)
Main Supervisor:
Engelbrecht, Kurt (Intern)
Examiner:
Jensen, Jens Oluf (Intern)
Kitanovski, Andrej (Ekstern)
Palm, Björn (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)

Relations
Publications:
Active magnetic regenerator refrigeration with rotary multi-bed technology
Project: PhD

Commercial project SOFC related

Department of Energy Conversion and Storage

Applied Electrochemistry
Period: 01/04/2016 → 31/03/2017
Number of participants: 1
Project participant:
Hagen, Anke (Intern)

Highly structured materials for upgraded biogas and storage
HiGradeGas will develop nanostructured materials for more efficient adsorption processes to remove CO₂ from biogas (upgrading) and to store the resulting biomethane.

Department of Energy Conversion and Storage
Ceramic Engineering & Science
SINTEF
Stockholm University
Syddansk Universitet
Danish Power Systems ApS
NeoZeo AB
Rambøll Oil and Gas
Luleå University of Technology
Period: 01/03/2016 → 29/02/2020
Number of participants: 1
Biogas upgrading, pressure swing adsorption, Nanofibers, gas adsorption
Acronym: HiGradeGas
Number of related Ph.D. students: 2
Project Coordinator:
Kaiser, Andreas (Intern)

Project

3D imaging center
Department of Physics
Neutrons and X-rays for Materials Physics
Department of Applied Mathematics and Computer Science
Image Analysis & Computer Graphics
Department of Energy Conversion and Storage
Imaging and Structural Analysis
Electrofunctional materials
Centre for oil and gas – DTU
Period: 01/01/2016 → 01/01/2021
Number of participants: 14
Project participant:
Dahl, Anders Bjorholm (Intern)
Oddershede, Jette (Intern)
Trinderup, Camilla Himmelstrup (Intern)
Simonsen, Søren Bredmose (Intern)
Zheng, Yi (Intern)
Brink, Bastian (Intern)
Lauridsen, Torsten (Ekstern)
Thydén, Karl Tor Sune (Intern)
Sanna, Simone (Intern)
Baier, Sina (Intern)
Bentzen, Janet Jonna (Intern)
Christensen, Anders Nymark (Intern)
Project Manager, organisational:
Gundlach, Carsten (Intern)
Project Manager, academic:
Poulsen, Henning Friis (Intern)

Relations
Related projects:
Alliance for Imaging and Modelling of Energy Applications
Publications:
From concept to in vivo testing: Microcontainers for oral drug delivery
Scene reassembly after multimodal digitization and pipeline evaluation using photorealistic rendering
Graphite nodules in fatigue-tested cast iron characterized in 2D and 3D
In-Situ X-ray Tomography Study of Cement Exposed to CO₂ Saturated Brine
Crack Tip Flipping under Mode I Tearing: Investigated by X-Ray Tomography
Powder embossing method for selective loading of polymeric microcontainers with drug formulation
High-Performance Microchanneled Asymmetric Gd₀.1Ce₀.9O₁.₉₅₋₅-La₀.₆Sr₀.₄FeO₃₋₅-Based Membranes for Oxygen Separation
Characterization of graphite nodules in thick-walled ductile cast iron
Surface Detection using Round Cut
Microstructure and micromechanics of the heart urchin test from X-ray tomography
Synthesis and characterization of Fe–Ni/γ-Al2O3 egg-shell catalyst for H2 generation by ammonia decomposition

High Temperature Superconducting Bolometer
Department of Energy Conversion and Storage
Electrofunctional materials
Department of Physics
Quantum Physics and Information Technology
Department of Photonics Engineering
Period: 01/01/2016 → 31/08/2016
Number of participants: 3
Superconductor
Supervisor:
Jepsen, Peter Uhd (Intern)
Main Supervisor:
Wulff, Anders Christian (Intern)

SOFC stack project
Department of Energy Conversion and Storage
Electrofunctional materials
Period: 01/01/2016 → 31/12/2016
Number of participants: 1
Project participant:
Wulff, Anders Christian (Intern)

New Thermoelectric Materials
Department of Energy Conversion and Storage
Electrofunctional materials
Period: 01/01/2016 → …
Number of participants: 1
Acronym: NeTeMa
Project Coordinator:
Van Nong, Ngo (Intern)

Thermal Energy Storage - Lab-Scale prototype
Large quantities of thermal energy - both per weight and price - can be stored reversibly in many salts upon ab-/desorption of water or ammonia. The project is to develop thermochemical heat storage (TCS) system based on NH3 ab/desorption in metal halides. We target for this lab-scale prototype a storage capacity of 1 MJ (2.5 kg NH3) based first on existing mixed metal salts (e.g. SrBaCl2), to demonstrate the system feasibility and document the actual efficiency of the different components and test the mechanical and structural properties of the system during multiple cycles.

Department of Energy Conversion and Storage
Atomic scale modelling and materials
Period: 01/01/2016 → 01/01/2018
Number of participants: 1
Thermal Energy Storage, Thermo chemical energy storage, ammonia
Acronym: TES
Project participant:
**High Efficiency Thermoelectric Module**

Department of Energy Conversion and Storage

Electrofunctional materials
- Period: 01/01/2016 → …
- Number of participants: 1
- Acronym: HiTEM
- Project Coordinator:
  - Van Nong, Ngo (Intern)

**Global Networking on Molecular Technology Research funded by JSPS (Japan)**

This is a network programme to support talented young researchers from Osaka University and Stanford University (USA), imec (Belgium, The Netherlands), Lawrence Berkeley National Laboratory (USA), Harvard University (USA), Utrecht University (The Netherlands), University of Bordeaux (France), Max Planck Institute, Mainz (Germany), Max Planck Institute, Stuttgart (Germany), University of Oxford (UK), Technical University of Denmark (Denmark), Forschungszentrum Jülich, GmbH (Germany), Carnegie Mellon University (USA), KU Lueven (Belgium), University of Southampton (UK)

Department of Energy Conversion and Storage

Ceramic Engineering & Science
- Period: 01/01/2016 → 31/12/2020
- Number of participants: 1
- Working partner:
  - Van Nong, Ngo (Intern)

**Development of a new synthesis for highly active fuel cell electrocatalysis**

Department of Energy Conversion and Storage
- Period: 15/12/2015 → 14/12/2018
- Number of participants: 4
- Phd Student:
  - Brandes, Benedikt Axel (Intern)
- Supervisor:
  - Cleemann, Lars Nilausen (Intern)
  - Li, Qingfeng (Intern)
- Main Supervisor:
  - Jensen, Jens Oluf (Intern)

**Financing sources**
- Source: Internal funding (public)
- Name of research programme: Institut stipendie (DTU)
- Project: PhD

**Improving the efficiency of heat pump and cooling technologies**

Department of Energy Conversion and Storage
- Period: 15/12/2015 → 14/12/2018
- Number of participants: 3
- Phd Student:
  - Navickaité, Kristina (Intern)
- Supervisor:
  - Bahl, Christian (Intern)
- Main Supervisor:
  - Engelbrecht, Kurt (Intern)

**Financing sources**
Development and characterization of emerging battery electrodes and electrolytes

Department of Energy Conversion and Storage
Period: 01/12/2015 → 30/11/2018
Number of participants: 4
Phd Student:
Lefevr, Jessica (Intern)
Supervisor:
Hoster, Harry Ernst (Ekstern)
Norby, Poul (Intern)
Main Supervisor:
Blanchard, Didier (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)

Relations
Activities:
Hydrides as Energy Materials
10th International Symposium "Hydrogen & Energy"
Lithium-Sulfur Solid-State Batteries Based on Nanoconfined LiBH4

Electrical Properties of Correlated Electron Systems at the Interfaces of Complex Oxides

Department of Energy Conversion and Storage
Period: 01/12/2015 → 30/06/2019
Number of participants: 4
Phd Student:
von Soosten, Merlin (Intern)
Supervisor:
Chen, Yunzhong (Intern)
Jespersen, Thomas Sand (Ekstern)
Main Supervisor:
Pryds, Nini (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Improvement of Electrode Materials for High temperature Electrolysis Cells

Department of Energy Conversion and Storage
Period: 01/12/2015 → 30/11/2018
Number of participants: 4
Phd Student:
Tripkovic, Dordije (Intern)
Supervisor:
Bilge, Yildiz (Ekstern)
Mogensen, Mogens Bjerg (Intern)
Main Supervisor:
Hendriksen, Peter Vang (Intern)

Financing sources
Source: Internal funding (public)
Next generation rechargeable batteries: Sustainable and earth-abundant materials

Department of Energy Conversion and Storage
Period: 01/12/2015 → 30/11/2018
Number of participants: 4
Phd Student:
Christensen, Mathias Kjærgård (Intern)
Supervisor:
Hoster, Harry Ernst (Ekstern)
Vegge, Tejs (Intern)
Main Supervisor:
Norby, Poul (Intern)

Financing sources
Source: Internal funding (public)

Name of research programme: Forskningsrådsfinansiering
Project: PhD

Improvement of Cell Strength in High Temperature Electrolysis Cells

Department of Energy Conversion and Storage
Period: 01/11/2015 → 31/10/2018
Number of participants: 3
Phd Student:
Khajavi, Peyman (Intern)
Supervisor:
Hendriksen, Peter Vang (Intern)
Main Supervisor:
Franelsen, Henrik Lund (Intern)

Financing sources
Source: Internal funding (public)

Name of research programme: Forskningsrådsfinansiering
Project: PhD

Durable thin ceramic films for improvement of Proton Exchange Membrane (PEM) electrolysis

Department of Energy Conversion and Storage
Period: 15/10/2015 → 14/10/2018
Number of participants: 4
Phd Student:
Fenini, Filippo (Intern)
Supervisor:
Kammer Hansen, Kent (Intern)
Hendriksen, Peter Vang (Intern)
Main Supervisor:
Mogensen, Mogens Bjerg (Intern)

Financing sources
Source: Internal funding (public)

Name of research programme: Forskningsrådsfinansiering
Project: PhD

Development of non-precious metal polymer fuel cell catalysts

Department of Energy Conversion and Storage
Period: 15/09/2015 → 14/12/2018
Number of participants: 4
Phd Student:
Shypunov, Illia (Intern)
Supervisor:
Cleemann, Lars Nilausen (Intern)
Li, Qingfeng (Intern)
Main Supervisor:
Jensen, Jens Oluf (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Modeling Energy Supply for Future Cities
Department of Energy Conversion and Storage
Period: 15/09/2015 → 14/09/2018
Number of participants: 7
Phd Student:
Dominkovic, Dominik Franjo (Intern)
Supervisor:
Nielsen, Per Sieverts (Intern)
Sørensen, Mads Peter (Intern)
Main Supervisor:
Pedersen, Allan Schrøder (Intern)
Examiner:
Jensen, Søren Højgaard (Intern)
Ahlgren, Erik (Intern)
Lund, Henrik (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet

Relations
Activities:
Blockchain Summer School 2017
Climate-KIC PhD Summer School Urban Transition Amsterdam-Bologna 2017
2018 MIT energy conference
12th International SDEWES Conference
Thermal building mass for storage and its role in smart energy systems
The 40th International IAEE Conference
National Renewable Energy Laboratory
30th International Conference on Efficiency, Cost, Optimization, Simulation and Environmental Impact of Energy Systems
Which storage types are needed in future smart energy cities?
Publications:
Potential for dynamic pricing in district heating systems in Denmark and Finland
Integration of district cooling in smart energy systems: the case of Singapore
Project: PhD

Nano-scale 3D reconstruction of phase contrast X-ray projections
Department of Energy Conversion and Storage
Period: 15/09/2015 → 14/09/2018
Number of participants: 3
Phd Student:
Cunha Ramos, Tiago Joao (Intern)
Supervisor:
Jørgensen, Jakob Sauer (Intern)
Main Supervisor:
Andreasen, Jens Wenzel (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

ESS & MAX IV: Cross border science and society
Workpackage: ESS & MAX IV: Cross border network and post graduate educational program

Department of Energy Conversion and Storage
Imaging and Structural Analysis
Department of Physics
Department of Applied Mathematics and Computer Science
University of Copenhagen
MaxLab
Lund University
Chalmers University of Technology
Malmö Högskola
European Spallation Source ESS AB
University of Oslo
University of Gothenburg
Aarhus University
Period: 01/09/2015 → 31/08/2018
Number of participants: 1
X-ray synchrotron scattering, neutron scattering
Project participant:
Kuhn, Luise Theil (Intern)

SOFC degradation studies
Department of Energy Conversion and Storage
Period: 15/08/2015 → 14/08/2018
Number of participants: 6
Phd Student:
Ploner, Alexandra (Intern)
Supervisor:
Hauch, Anne (Intern)
Main Supervisor:
Hagen, Anke (Intern)
Examiner:
Graves, Christopher R. (Intern)
Himanen, Olli Pekka (Ekstern)
Weber, André (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet
Project: PhD

Development and characterization of novel high temperature and pressure alkaline electrolysis cells (HTP-AEC)
Department of Energy Conversion and Storage
Development and characterization of novel high temperature and pressure alkaline electrolysis cells (HTP-AEC)

Department of Energy Conversion and Storage
Period: 01/08/2015 → 31/08/2018
Number of participants: 4
PhD Student:
Adolphsen, Jens Quitzau (Intern)
Supervisor:
Chatzichristodoulou, Christodoulos (Intern)
Gil, Vanesa (Intern)
Main Supervisor:
Sudireddy, Bhaskar Reddy (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Multilayer inorganic structures for high performance enzyme immobilization and separation

Department of Energy Conversion and Storage
Period: 01/08/2015 → 30/11/2015
Number of participants: 4
PhD Student:
Ghannadi, Saber (Intern)
Supervisor:
Kaiser, Andreas (Intern)
Pinelo, Manuel (Intern)
Main Supervisor:
Della Negra, Michela (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Dark Field X-ray Microscopy of energy materials

Department of Energy Conversion and Storage
Period: 15/06/2015 → 14/07/2018
Number of participants: 7
PhD Student:
Sierra Trujillo, Jose Xavier (Intern)
Supervisor:
Jørgensen, Peter Stanley (Intern)
Poulsen, Henning Friis (Intern)
Main Supervisor:
Bowen, Jacob R. (Intern)
Examiner:
Hagen, Anke (Intern)
Sørensen, Henning Osholm (Intern)
Villanova, Julie (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet

Relations
Activities:
Sample Design and Preparation Techniques for Dynamic Microstructural Studies of High Temperature Electrochemical Cells
Project: PhD

Durable thin ceramic films for improvement of Proton Exchange Membrane (PEM) electrolysis cells

Department of Energy Conversion and Storage
Period: 15/06/2015 → 31/07/2015
Number of participants: 4
Phd Student:
Hausladen, Mathias (Intern)
Supervisor:
Hendriksen, Peter Vang (Intern)
Ramos, Tania (Intern)
Main Supervisor:
Mogensen, Mogens Bjerg (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Electrochemical Characterization for Improvement of PEM Electrolysers for Flexible Energy Storage

Department of Energy Conversion and Storage
Period: 15/06/2015 → 14/06/2018
Number of participants: 7
Phd Student:
Elsøe, Katrine (Intern)
Supervisor:
Hjelm, Johan (Intern)
Main Supervisor:
Mogensen, Mogens Bjerg (Intern)
Examiner:
Hauch, Anne (Intern)
Hauch, Anne (Intern)
Sunde, Svein (Ekstern)
Sunde, Svein (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

High Current All Printed Transistors
The fast evolution of printed electronics, with the photovoltaic technology in primis, is requiring the presence of a valid transistor alternative to the traditional one. The realization of a high current roll-to-roll transistor will interconnect all the different technologies so far developed with this low cost and high throughput method. Our
aim is to develop a roll-to-roll transistor capable of modulating the current to levels that have not been achieved so far. The fabrication of the transistor will be done considering the lowest environmental impact possible, and containing energy consumption with a temperature below 150 °C. This high current (~mA) transistor will be able to support and assist other technologies and will also be the base for logics and sensing application.

The optical studies on the organic material will result in a more controllable production process that for the first time will relate polymer crystallinity directly with an optical characterization technique. The realization of such kind of measurements is not trivial, but will give information on polymer nanoscale structures never investigated before. To do so this technique uses femtosecond pulse in subdiffraction-limited area. This will disclose an unprecedented tool to control the polymer morphology as soon as it is deposited, with enormous consequences in performance control and optimization.

The realization of samples and the study of real cases will produce important information regarding this new technology and its real life applications. In addition, life-time and stability studies can be performed. Then the objective of minimizing the environmental impact of the technology life cycle will be more realistic. These kinds of studies are also important to explain science to the society and to give a technology preview to industries.

Department of Energy Conversion and Storage

Organic Energy Materials
Period: 01/05/2015 → ...
Number of participants: 1
printed, electronics, smart, windows, Solar Cells, Organic
Acronym: HCAPT
Project ID: 659747
Project participant:
Pastorelli, Francesco (Intern)
Documents:
European Commission _ CORDIS _ Projects and Results _ High Current All Printed Transistors Project

New composite materials for high temperature water splitting and synthetic fuel production by solar thermochemical conversion

In this project we propose a novel concept material for high temperature H2O/CO2 splitting based on a porous ceramic composite comprised of high-temperature ceramics and cerium oxide in its highly doped form. In the composite, the low diffusivity at the refractory component inhibits the mass diffusion mechanisms in the catalytic component (doped-ceria), thus preserving the microstructure from the detrimental densification effects.

Department of Energy Conversion and Storage

Ceramic Engineering & Science
Period: 01/05/2015 → 31/03/2018
Number of participants: 1
Acronym: HT-COMPO
Project Coordinator:
Esposito, Vincenzo (Intern)
Project

In-operando spatially resolved probing of solid oxide electrolysis/fuel cells

Department of Energy Conversion and Storage

Period: 01/05/2015 → 30/04/2018
Number of participants: 8
Phd Student:
Pitscheider, Simon (Intern)
Supervisor:
Chueh, William C. (Ekstern)
Hansen, Karin Vels (Intern)
Hjelm, Johan (Intern)
Main Supervisor:
Chatzichristodoulou, Christodoulos (Intern)
Examiner:
Hendriksen, Peter Vang (Intern)
Fleig, Jürgen (Ekstern)
Knudsen, Jan (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering

**Relations**
Publications:
In-operando spatially resolved probing of solid oxide electrolysis/fuel cells
Project: PhD

**Young investigator Program from Villum Foundation**
Department of Energy Conversion and Storage
Period: 01/05/2015 → 07/01/2019
Number of participants: 4
Phd Student:
Mathiesen, Nicolai Rask (Intern)
Supervisor:
Vegge, Tejs (Intern)
Vegge, Tejs (Intern)
Main Supervisor:
García Lastra, Juan Maria (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Eksternt finansieret virksomhed
Project: PhD

**SOFC Testing Part 1 and 2**
Department of Energy Conversion and Storage
Applied Electrochemistry
Period: 13/04/2015 → 31/10/2015
Number of participants: 2
Project participant:
Hagen, Anke (Intern)
Sun, Xiufu (Intern)

**Density Functional Theory Studies of the Oxygen Reduction Reaction on Non-Precious Electrodes**
Department of Energy Conversion and Storage
Period: 01/04/2015 → 20/06/2018
Number of participants: 6
Phd Student:
Reda, Mateusz Krzysztof (Intern)
Supervisor:
Hansen, Heine Anton (Intern)
Main Supervisor:
Vegge, Tejs (Intern)
Examiner:
Cleemann, Lars Nilausen (Intern)
Groß, Axel (Ekstern)
Skulason, Egill (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD
In-operando localized probing of solid oxide electrolysis/fuel cells by controlled atmosphere high temperature scanning probe microscopy

Department of Energy Conversion and Storage
Period: 15/03/2015 → 14/06/2018
Number of participants: 8
Phd Student:
Kreka, Kosova (Intern)
Supervisor:
Chatzichristodoulou, Christodoulos (Intern)
Mogensen, Mogens Bjerg (Intern)
Norman, Kion (Intern)
Main Supervisor:
Hansen, Karin Vels (Intern)
Examiner:
Hjelm, Johan (Intern)
Bieberle-Hüter, Anja (Ekstern)
Küngas, Rainer (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

The role of contact resistance in thermoelectric module

Department of Energy Conversion and Storage
Period: 15/02/2015 → 01/08/2018
Number of participants: 6
Phd Student:
Malik, Safdar Abbas (Intern)
Supervisor:
Stamate, Eugen (Intern)
Main Supervisor:
Van Nong, Ngo (Intern)
Examiner:
Kaiser, Andreas (Intern)
Pryds, Nini (Intern)
Rezaniakolaei, Alireza (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Demonstration of Danmarks Fremtidige Energisystem in Miniformat

Department of Energy Conversion and Storage
Applied Electrochemistry
Period: 19/01/2015 → 31/12/2015
Number of participants: 1
Project participant:
Hagen, Anke (Intern)

Filamentary Coated Conductors
Internal DTU Energy project about superconducting tapes;
Main objective is to develop a strongly cube textured two-level-undercut-profile-substrate for filamentary coated conductors.
Rare-earth/transition-metal oxides and compounds for environment-friendly energy science and technology
This network programme is to setup win-win scientific collaborations between the DTU Energy Conversion and the State Key Laboratory of Magnetism (SKLM), Institute of Physics (IOP), Chinese Academy of Sciences (CAS) in Beijing, China. This is expected to improve largely the core competences for both the Danish and the Chinese partners, known for advanced energy conversion technology and excellent fundamental research, respectively.

Acid-base chemistry and HT-polymer electrolyte membranes

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Advanced nano-inks for ink-jet printing of functional metal oxides for energy and environment devices - Smart Inks
Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)

Relations
Publications:
Smart nano-inks for inkjet printing of functional oxide based thin films
Project: PhD

ECOdesign of urban buildings by integration of organic photovoltaics microgrids (ECLIPS microgrids)
Department of Energy Conversion and Storage
Period: 15/12/2014 → 22/05/2018
Number of participants: 7
Phd Student:
Chatzisideris, Marios Dimos (Intern)
Supervisor:
Gevorgyan, Suren (Intern)
Main Supervisor:
Laurent, Alexis (Intern)
Examiner:
Owsianiak, Mikolaj (Intern)
Owsianiak, Mikolaj (Intern)
Nelson, Jenny (Ekstern)
Nelson, Jenny (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet
Project: PhD

Analysis of Fracture in Porous Ceramic Catalysts by use of X-ray Tomography
Department of Energy Conversion and Storage
Period: 01/12/2014 → 11/07/2018
Number of participants: 5
Phd Student:
Jacobsen, Hjalte Sylvest (Intern)
Supervisor:
Molina, Anna M. Puig (Ekstern)
Paulsen, Henning Friis (Ekstern)
Sørensen, Bent F. (Intern)
Main Supervisor:
Frandsen, Henrik Lund (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Development of High temperature PEM fuel cells
Department of Energy Conversion and Storage
Period: 15/11/2014 → 14/11/2017
Number of participants: 5
Phd Student:
Kannan, Arvind (Intern)
Main Supervisor:
Jensen, Jens Oluf (Intern)
Examiner:
Bjerrum, Niels J. (Intern)
Andreasen, Søren Juhl (Ekstern)
Zeis, Roswitha (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Offentlig finansiering
Project: PhD

**Topology optimization of thermal heat sinks**
PhD Project
Department of Energy Conversion and Storage
Electrofunctional materials
Department of Mechanical Engineering

Solid Mechanics
Period: 01/11/2014 → 31/10/2017
Number of participants: 4
Acronym: TOPTEN
Project participant:
Engelbrecht, Kurt (Intern)
Sigmund, Ole (Intern)
Lazarov, Boyan Stefanov (Intern)
Phd Student:
Haertel, Jan Hendrik Klaas (Intern)

**Relations**
Publications:
Topology Optimization of Thermal Heat Sinks

**In situ transmission electron microscopy on operating electrochemical cells**
Solid oxide fuel/electrolysis cells (SOFC/SOEC) will play an important role in future efficient and environmentally friendly energy systems if a better long term performance of the cells can be achieved. In a solid oxide fuel cell (SOFC) a fuel such as hydrogen, methane, synthesis gas, etc. is oxidized over a solid oxygen ion-conducting electrolyte which physically

**Financing sources**
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering

**Relations**
Publications:
Design of Thermal Systems Using Topology Optimization
Project: PhD
separates fuel and air.

The electron transfer in this chemical reaction takes place via an external circuit and electricity is therefore a product of the reaction. Catalysts are used on both sides of the ion conducting electrolyte to activate the splitting of fuel and oxygen molecules.

Impressive performance improvements have recently been reported for cells with specific multiphase nano-structures, but structural and compositional nano-scaled changes can also lead to deactivation. On the other hand, deactivation processes due to nano-scaled structural and compositional changes (segregations followed by nano-particle precipitation in some cases) can be observed near the material interfaces in the electrodes. Neither the mechanisms of the initial fast electrode process nor the development and dynamics of these critical structures are understood. Further studies of these dynamical changes are hampered since there are no available methods which offer in situ characterization of operating cells with nano-scale spatial resolution.

The project will develop a method for in situ transmission electron microscopy (TEM) of operating solid oxide electrochemical cells. Until now, knowledge of the nanoscale SOFC/SOEC dynamics is entirely based on observations performed post mortem, when the cells have been cooled down and de-mounted. To obtain direct insight into the dynamics of the active nanostructures of a SOFC/SOEC in operation can therefore have significant importance for our understanding of the cell dynamics during activation and deactivation.

The aim is to record TEM image sequences (movies) with atomic resolution of the active nanostructures in the SOFC/SOEC during operation. To do this, model SOFC/SOEC systems will be developed and integrated into a TEM holder so that heating, electrical currents and exposure to reactive gas environments all are integrated at the same time. In addition the model systems will need to be highly compact and the thickness of the imaged area should be approximately 100 nm. The project will therefore push the limits of in situ TEM experiments.

The goal is direct insight into the nano-scale dynamics of the operating SOFC/SOEC during exposure to elevated temperatures, electrical currents and a reactive gas environment. This will be a key factor in developing more efficient and stable SOFCs/SOECs. Therefore, micro-SOFC will be developed and characterized by thin layer, especially regarding the electrolyte layer which will have a thickness lower than one micrometre. This will allow to work at temperature lower than 600°C.

The project will be carried out as a PhD project in collaboration between the two applicant institutions (DTU Energy Conversion and DTU Cen) and with the in situ group from Nagoya University with Prof. Shunsuke Muto. The work will primarily be carried out by the PhD student with support and supervision from the project team. The principal supervisor is Head of Section Luise T. Kuhn. The TEM work will be carried out under the guidance of Søren Bredmose Simonsen and Prof. Jakob B. Wagner. Prof. Mogens B. Mogensen will contribute to the project as an internal consultant when analyzing and linking the observed physical properties to the electrochemical performance.

Department of Energy Conversion and Storage

Imaging and Structural Analysis

Center for Electron Nanoscopy

DTU Danchip
Period: 01/10/2014 → 30/09/2017
Number of participants: 4
In-situ TEM, fuel cell, electrolysis, electrochemistry, Nanotechnology
Acronym: TEMOC
Number of related Ph.D. students: 1
Project participant:
Kuhn, Luise Theil (Intern)
Simonsen, Søren Bredmose (Intern)
Wagner, Jakob Birkedal (Intern)
Gualandris, Fabrizio (Intern)
Project

In-situ transmission electron microscopy on operating electrochemical cells

Department of Energy Conversion and Storage
Period: 01/10/2014 → 24/01/2018
Number of participants: 7
Phd Student:
Gualandris, Fabrizio (Intern)
Graded Oxygen Transport Membranes for Carbon Capture Processes

Department of Energy Conversion and Storage
Period: 15/09/2014 → 24/01/2018
Number of participants: 7
Phd Student:
Pirou, Stéven (Intern)
Supervisor:
Hendriksen, Peter Vang (Intern)
Kaiser, Andreas (Intern)
Main Supervisor:
Kiebach, Wolff-Ragnar (Intern)
Examiner:
Agersted, Karsten (Ekstern)
Baumann, Stefan (Ekstern)
Kriegel, Ralf (Ekstern)

Financial sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Studies of doping effects on the superconducting properties of DyBa2Cu2O7-d and its possible manufacture as thin film for power applications

Department of Energy Conversion and Storage
Period: 01/09/2014 → 18/04/2018
Number of participants: 7
Phd Student:
Opata, Yuri Aparecido (Intern)
Supervisor:
Hansen, Jern Otto Bindslev (Ekstern)
Yue, Zhao (Intern)
Main Supervisor:
Grivel, Jean-Claude (Intern)
Examiner:
Chen, Yunzhong (Intern)
Crisan, Ioan Adrian (Ekstern)
Obradors, Xavier (Ekstern)

Financial sources
In-situ 3D microstructure characterisation of solid oxide fuel cells using X-ray tomography methods

Department of Energy Conversion and Storage
Period: 15/08/2014 → 13/12/2017
Number of participants: 7
PhD Student:
De Angelis, Salvatore (Intern)
Supervisor:
Jørgensen, Peter Stanley (Intern)
Lauridsen, Erik Mejdal (Intern)
Main Supervisor:
Bowen, Jacob R. (Intern)
Examiner:
Andreasen, Jens Wenzel (Intern)
Carbone, Gerardina (Ekstern)
Chiu, Wilson K. S. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering

Relations
Activities:
Wilson K. S. Chiu
Gerardina Carbone
Sample Design and Preparation Techniques for Dynamic Microstructural Studies of High Temperature Electrochemical Cells
Publications:
Tracking Solid Oxide Cell Microstructure Evolution by High Resolution 3D Nano-Tomography
Project: PhD

Robust HT-MEAs for Dynamic Operation under Smart Grid Conditions

Department of Electrical Engineering
Center for Electric Power and Energy
Distributed Energy Resources
Department of Energy Conversion and Storage
Proton conductors
Period: 01/08/2014 → 01/08/2017
Number of participants: 3
Acronym: SmartMEA
Project participant:
Pensini, Alessandro (Intern)
Træholt, Chresten (Intern)
Project Manager, organisational:
Jensen, Jens Oluf (Intern)
Project

Alkaline Electrolyser Cell

Department of Energy Conversion and Storage
Period: 01/08/2014 → 13/11/2017
Number of participants: 8
PhD Student:
Kraglund, Mikkel Rykær (Intern)
Supervisor:
Aili, David (Intern)
Jensen, Jens Oluf (Intern)
Nikiforov, Aleksey Valerievich (Intern)
Main Supervisor:
Christensen, Erik (Intern)
Examiner:
Chatzichristodoulou, Christodoulos (Intern)
Sunde, Svein (Ekstern)
Therkildsen, Kasper Tipsmark (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)

**Relations**
Publications:
Alkaline membrane water electrolysis with non-noble catalysts
Project: PhD

**Roll-to-roll X-ray scattering and analysis**
Department of Energy Conversion and Storage
Period: 01/08/2014 → 26/01/2019
Number of participants: 3
Phd Student:
Rossander, Lea Hildebrandt (Intern)
Supervisor:
Trofod, Thue (Intern)
Main Supervisor:
Andreasen, Jens Wenzel (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet
Project: PhD

**Solid oxide fuel cells for the renewable energy transition**
Project nr 2014-1-12231 funded by Energinet.dk’s ForskEL programme
Department of Energy Conversion and Storage
Applied Electrochemistry
Period: 01/08/2014 → 31/03/2017
Number of participants: 1
electrochemistry, solid oxide fuel cells , SOFC
Acronym: SOFC4RET
Number of related Ph.D. students: 3
Project Manager, academic:
Graves, Christopher R. (Intern)

**CHEETAH FP7**
CHEETAH - Cost-reduction through material optimisation and Higher EnErgy outpuT of solAr pHotovoltaic modules -
joining Europe’s Research and Development efforts in support of its PV industry - is a combined collaborative project (CP)
and coordination and support action (CSA) funded under the European Commission’s 7th Framework programme.
CHEETAH’s aims to solve specific R&D issues in the EERA-PV Joint Program and to overcome fragmentation of
European PV R&D in Europe and intensify the collaboration between R&D providers and industry to accelerate the
industrialization of innovations.
Department of Energy Conversion and Storage
Functional organic materials
Period: 21/07/2014 → …
Number of participants: 1
Project participant:
Beliatis, Michail (Intern)

**Green Production of Nanomaterials for Energy Conversion**
Department of Energy Conversion and Storage
Period: 01/07/2014 → 30/09/2017
Number of participants: 8
Phd Student:
Xu, Yu (Intern)
Supervisor:
Hendriksen, Peter Vang (Intern)
Norby, Poul (Intern)
Simonsen, Søren Bredmose (Intern)
Main Supervisor:
Kiebach, Wolff-Ragnar (Intern)
Examiner:
Della Negra, Michela (Intern)
Aymonier, Cyril (Ekstern)
Lester, Edward Henry (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering

**Relations**
Publications:
Continuous Hydrothermal Flow Synthesis of Functional Oxide Nanomaterials Used in Energy Conversion Devices
Project: PhD

**Electrochemical Reduction of CO2 to Sustainable Synthetic Fuels**
Department of Energy Conversion and Storage
Period: 01/06/2014 → 20/09/2017
Number of participants: 6
Phd Student:
Bhowmik, Arghya (Intern)
Supervisor:
Hansen, Heine Anton (Intern)
Main Supervisor:
Vegge, Tejs (Intern)
Examiner:
Norby, Poul (Intern)
Skulason, Egill (Intern)
Studt, Felix (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet

**Relations**
Publications:
Design of oxide electrocatalysts for efficient conversion of CO2 into liquid fuels
Project: PhD
Electrospun functionalized nano-materials for ultra-compact de-NOX SCR system in naval shipping

Department of Energy Conversion and Storage
Ceramic Engineering & Science
Period: 01/05/2014 → 01/07/2016
Number of participants: 1
Acronym: BLUESHIP
Project ID: 605102
Project participant:
Esposito, Vincenzo (Intern)

Development of Proton Conductive membranes
Department of Energy Conversion and Storage
Period: 01/05/2014 → 09/07/2017
Number of participants: 7
Phd Student:
Kirkebæk, Andreas (Intern)
Supervisor:
Aili, David (Intern)
Jensen, Jens Oluf (Intern)
Main Supervisor:
Li, Qingfeng (Intern)
Examiner:
Søndergaard, Roar R. (Intern)
Hjuler, Hans Aage (Intern)
Kerres, Jochen (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Lifetime limiting effects in pre-commercial solid cell devices
Department of Energy Conversion and Storage
Period: 01/03/2014 → 21/06/2017
Number of participants: 7
Phd Student:
Skafte, Theis Løye (Intern)
Supervisor:
Blennnow Tullmar, Peter (Intern)
Graves, Christopher R. (Intern)
Main Supervisor:
Hjelm, Johan (Intern)
Examiner:
Hauch, Anne (Intern)
Lanzini, Andrea (Ekstern)
Weber, André (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Industrial PhD

Relations
Publications:
Lifetime limiting effects in pre-commercial solid oxide cell devices
Project: PhD
Inks for fast processing of recyclable polymer solar cells

Department of Energy Conversion and Storage
Period: 15/01/2014 → 26/04/2017
Number of participants: 5
Phd Student:
Benatto, Gisele Alves dos Reis (Intern)
Main Supervisor:
Krebs, Frederik C (Intern)
Examiner:
Andreasen, Jens Wenzel (Intern)
Tanenbaum, David M. (Ekstern)
Wang, Ergang (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Offentlig finansiering

Relations
Publications:
Large scale roll-to-roll produced organic photovoltaic devices: manufacturing, lifetime and environmental impact
Project: PhD

Alliance for Imaging and Modelling of Energy Applications
The CINEMA research alliance will develop unique 3D micro-structural characterization methods, which make it possible to investigate components under realistic conditions and in real time. This will enable correlation between performance and local changes in the microstructure.

Department of Energy Conversion and Storage
Imaging and Structural Analysis
Department of Physics
Neutrons and X-rays for Materials Physics
Department of Wind Energy
Composites and Materials Mechanics
Department of Applied Mathematics and Computer Science
Image Analysis & Computer Graphics
Scientific Computing
Mixed Conductors
Statistics and Data Analysis
University of Copenhagen
Northwestern University
University of Manchester
MaxLab
LM Wind Power
Haldor Topsoe AS
Xnovo Technology ApS
Rockwool International
Amminex Emissions Technology A/S
Period: 01/01/2014 → 31/12/2018
Number of participants: 26
Acronym: CINEMA
Project participant:
Mikkelsen, Lars Pilgaard (Intern)
Sørensen, Bent F. (Intern)
Bowen, Jacob R. (Intern)
Kuhn, Luise Theil (Intern)
Larsen, Rasmus (Intern)
Hansen, Per Christian (Intern)
Frandsen, Henrik Lund (Intern)
Gundlach, Carsten (Intern)
Dahl, Anders Bjorholm (Intern)
Yang, Shu-Yi (Intern)
Poulsen, Stefan Othmar (Intern)
Lyckegaard, Allan (Intern)
Lauridsen, Erik Mejdal (Intern)
Sørensen, Henning Osholm (Ekstern)

Project Manager, organisational:
Sørensen, Hanne (Intern)
Phd Student:
Jespersen, Kristine Munk (Intern)
Beil, Johannes (Ekstern)
Andersen, Michael (Intern)
Emerson, Monica Jane (Intern)
De Angelis, Salvatore (Intern)
Birkelund, Klaus (Ekstern)
Jacobsen, Hjalte Sylvest (Intern)
Chapelle, Lucie (Intern)
Supervisor:
Frandsen, Henrik Lund (Intern)
Project Manager, academic:
Andreasen, Jens Wenzel (Intern)
Project Coordinator:
Poulsen, Henning Friis (Intern)

Relations
Activities:
DTU Energy Conversion 2nd International PhD Summer School
Wilson K. S. Chiu
High resolution ptychographic tomography of soft matter
Gerardina Carbone
Sample Design and Preparation Techniques for Dynamic Microstructural Studies of High Temperature Electrochemical Cells
DTU Energy Conversion 2nd International PhD Summer School
Publications:
Fatigue damage evolution in fibre composites for wind turbine blades
Micromechanical Time-Lapse X-ray CT Study of Fatigue Damage in Uni-Directional Fibre Composites
Improving organic tandem solar cells based on water-processed nanoparticles by quantitative 3D nanoimaging
Micromechanical Investigation of Fatigue Damage in Uni-Directional Fibre Composites
Dictionary Based Segmentation in Volumes
3D X-Ray Computed Tomography (XCT) of Fatigue Damage Evolution in UD Glass Fibre Composite
Enabling Flexible Polymer Tandem Solar Cells by 3D Ptychographic Imaging

Project

Noble Metals Free Intermediate -Temperature Supported Liquid Phase Electrolyzer
The strategic development of the NobleFree project is noble metal free intermediate-temperature (200-400 C) fuel cells and water electrolyser with the same characteristics as of the Nafion®, PBI and Aquivion™ systems. This goal will be achieved by use of alkaline metals dihydrogen phosphates as proton-conducting supported liquid phase electrolytes (SLPE). These electrolytes will be liquid immobilized on ceramic nano fibers, whiskers and powders. It has been discovered recently, that nickel, high-nickel alloys and austenitic stainless steels containing small amounts of Ti have high
corrosion resistance in the molten alkali metals dihydrogen phosphates in the above mentioned temperature range. The NobleFree will start with the parallel development of electrolytes and nickel-based catalysts. The final stage of the project will be design and test of noble metal free intermediate temperature water electrolyser. Possibilities of use SLPE system as a fuel cell will be also studied.

Department of Energy Conversion and Storage

Proton conductors

Energy and Materials
Period: 01/01/2014 → ...
Number of participants: 5
Acronym: Noble Free
Project participant:
Nikiforov, Aleksey Valerievich (Intern)
Bjerrum, Niels J. (Intern)
Petrushina, Irina (Intern)
Christensen, Erik (Intern)
Jensen, Jens Oluf (Intern)

Sustainable Carbon Power
SUCAP eller ("Grøn Kulkraft") handler om at fremstille ikke-fossilt kulstof til kombineret energilagring og CO2 fjernelse. Den centrale idé i SUCAP projektet er at konvertere kombinationen af elektrisk vedvarende energi og CO2 til kombinationen af kul og oxygen, altså til et lager af potentiel energi. Processen er absolut mulig rent kemisk, men ikke udviklet og afprøvet, idet den hidtil været anset som ineffektiv og uadgivelig til energilagring. Vi vil vise, at det er muligt og effektivt at lagre energi som kul. SUCAP handler primært om at reducere CO2 til kul, d.v.s. da fuldstændige omdannelse, men det er også muligt at forhindre et partielle CO2 reduktion til f.eks. brændstofferne kulmonoxid (CO), metan (CH4), dimethyl ether (DME), methanol (CH3OH) og andre flydende energistoffer. Projektet har som opgave at udvikle metoder hertil og demonstrere gennemførelse af processen i praksis, samt at vurdere økonomien. Hvis effektiviteten kan blive rimelig, hvad vi tror, kan projektet få meget vidtrækkende betydning for samfundets energiforsyning.

Department of Chemistry

Department of Energy Conversion and Storage
Period: 01/01/2014 → 31/08/2018
Number of participants: 2
carbondioxide , carbon-capture , electricity-load-leveling, energy , environment
Acronym: SUCAP
Project participant:
Berg, Rolf W. (Intern)
Project applicant:
Bjerrum, Niels J. (Intern)

Center for IT-Intelligent Energy Systems for Cities
A wide range of research activities have arisen to support the Danish target of a 100% renewable energy system by 2050. Projects focused on individual aspects of the energy system, such as zero emissions buildings or intelligent power systems provide valuable insight, that facilitates flexibility throughout the energy system. CITIES will address this deficiency by establishing an integrated research centre covering all aspects of the energy system, including gas, power, district heating/cooling and biomass, and most importantly methods to forecast, control and optimize their interactions through the use of advanced ICT solutions.

The high densities of population, energy consumption, and energy and communications networks in cities offer the greatest potential for flexibility at the last cost, and the fact that cities account for 80% of global energy consumption and emissions [1] make the urban environment an ideal setting for energy systems integration research. CITIES will pioneer research into fully integrated city energy systems, building short-term operational models that feed longer term planning models, considering the spatiotemporal variations, interactions, dynamics and stochastics in the energy system. Low level models of system components will inform higher-level aggregate models employed in market and control framework design. The leading position of European academia and industry and the rapidly growing market for smart energy solutions indicates substantial scope for increased competitiveness and job creation within this field. CITIES will, in collaboration with its industrial and academic partners, conduct research with a view to developing tools for the implementation of integrated energy system solutions.

Center granted by Strategic Research Council.
To be a sustainable organisation.

Department of Applied Mathematics and Computer Science
Department of Civil Engineering
Department of Management Engineering
Department of Energy Conversion and Storage
Department of Informatics and Mathematical Modeling
Centre for IT-Intelligent Energy Systems in Cities

Aalborg University
Period: 01/01/2014 → 31/12/2019
Number of participants: 8

Strategic
Acronym: CITIES
Number of related Ph.D. students: 12
Project participant:
Madsen, Henrik (Intern)
Heller, Alfred (Intern)
Nielsen, Per Sieverts (Intern)
Pedersen, Allan Schrøder (Intern)
Rode, Carsten (Intern)
Pinson, Pierre (Intern)
Jørgensen, John Bagterp (Intern)
Project Manager, organisational:
Herrmann, Ivan Tengbjerg (Intern)

Financing sources
Source: Forskningsrådene - Andre
Name of research programme: Energy Programme
Amount: 44.00 Danish Kroner
Year of approval: 2013

Relations
Activities:
Blockchain Summer School 2017
Climate-KIC PhD Summer School Urban Transition Amsterdam-Bologna 2017
CITIES Annual Conference
3rd International Workshop on Design in Civil and Environmental Engineering
2018 MIT energy conference
Executive Development Programme with Technical University of Denmark
12th International SDEWES Conference
Energy Supply Modelling in Cities: Illustrated Using Data from the Danish Municipality of Sønderborg
Energy Supply Modelling in Cities: Illustrated Using Data from the Case of Sønderborg
Big Data som værktøj til at styre byens energi
Thermal building mass for storage and its role in smart energy systems
The 40th International IAEE Conference
National Renewable Energy Laboratory
Big Data as a tool for controlling the cities energy: Data aspects and data management
30th International Conference on Efficiency, Cost, Optimization, Simulation and Environmental Impact of Energy Systems
Which storage types are needed in future smart energy cities?
Status and Results of Energy Supply Modelling in CITIES: Illustrated using Data from the Case of Sønderborg

Publications:
Model Identification for Control of Display Units in Supermarket Refrigeration Systems
Center for Thermoelectric Energy Conversion
Department of Energy Conversion and Storage

Electrofunctional materials
Period: 01/01/2014 → 31/12/2018
Number of participants: 1
Acronym: CTEC
Working partner:
Van Nong, Ngo (Intern)

Elektrode Kinetics and Gas Conversion in Solid Oxide Cells
Department of Energy Conversion and Storage
Period: 01/01/2014 → 20/04/2016
Number of participants: 7
Phd Student:
Njodzefon, Jean-Claude (Intern)
Supervisor:
Graves, Christopher R. (Intern)
Weber, André (Ekstern)
Main Supervisor:
Hjelm, Johan (Intern)
Examiner:
Hauch, Anne (Intern)
Krügel, Albert (Ekstern)
Schefold, Josef (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Eksternt finansieret virksomhed

Relations
Publications:
Electrode Kinetics and Gas Conversion in Solid Oxide Cells
Project: PhD

Elektrokatalyse og Katalysatorer til Oxygenreduktion i Polymer Brændselscelle
Department of Energy Conversion and Storage
Period: 01/01/2014 → 17/05/2017
Number of participants: 7
Phd Student:
Zhong, Lijie (Intern)
Supervisor:
Cleemann, Lars Nilausen (Intern)
Jensen, Jens Oluf (Intern)
Main Supervisor:
Li, Qingfeng (Intern)
Examiner:
Bjerrum, Niels J. (Intern)
Steenberg, Thomas (Intern)
Steenberg, Thomas (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering

Relations
Publications:
Graphitic Layer Encapsulated Iron Based Non-precious Catalysts for the Oxygen Reduction Reaction
Materials for Energy Production

Department of Energy Conversion and Storage
Period: 01/01/2014 → 26/04/2017
Number of participants: 5
Phd Student:
Heckler, Ilona Maria (Intern)
Main Supervisor:
Bundgaard, Eva (Intern)
Examiner:
Andreasen, Jens Wenzel (Intern)
Tanenbaum, David M. (Ekstern)
Wang, Ergang (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Offentlig finansiering

Relations
Publications:
Polymer materials for roll coated solar cells: strategies tom improve performance and stability
Project: PhD

Nano-carbons for versatile power supply modules
NanoCaTe, a project co-financed by the European Commission, is focused on innovative flexible thermoelectric materials, based on standard and modified nanocarbon materials like graphene or carbon nanotubes. Twelve partners from Austria, Denmark, Finland, Germany, and Spain develop materials for thermoelectric energy harvesting and energy storage for manifold applications like pulsed sensors or mobile electronic devices.
The integration of the developed materials into harvester and storage devices is a further step to characterize the performance of the innovative materials.
Finally, a demonstrator consisting of harvester, storage and energy management represents a self-sustaining, universally usable, and maintenance-free power supply.
The project strengthens the position of Europe in the field of thermoelectric and storage materials by developing devices with increased lifetime produced by cost-efficient technologies and therefore contributing to a further promotion of cleaner energy technologies.
For detailed information visit http://nanocate.eu/

Department of Energy Conversion and Storage
Electrofunctional materials
Period: 01/12/2013 → 30/09/2017
Number of participants: 1
NanoCaTe
Project Manager, academic:
Van Nong, Ngo (Intern)

Financing sources
Source: Public research council
Name of research programme: 7th Framework Programme for Research and Technological Development
Amount: 4,900,000.00 Euro

Organic based photovaltaics with morphological control
Department of Energy Conversion and Storage
Period: 01/10/2013 → 30/06/2015
Number of participants: 3
Phd Student:
Zawacka, Natalia Klaudia (Intern)
Supervisor:
Krebs, Frederik C (Intern)
Main Supervisor:
Jørgensen, Mikkel (Intern)

Financial sources
Source: Internal funding (public)
Name of research programme: Grundforskningsfonden
Project: PhD

Active Cooling of a Down Hole Well Tractor
Department of Energy Conversion and Storage
Period: 01/09/2013 → 16/11/2016
Number of participants: 7
Phd Student:
Soprani, Stefano (Intern)
Supervisor:
Bahl, Christian (Intern)
Nesgaard, Carsten (Intern)
Main Supervisor:
Engelbrecht, Kurt (Intern)
Examiner:
Van Nong, Ngo (Intern)
Veje, Christian T. (Ekstern)
Verda, Vittorio (Ekstern)

Financial sources
Source: Internal funding (public)
Name of research programme: ErhvervsPhD-ordningen VTU

Relations
Publications:
Active cooling of a down hole well tractor
Project: PhD

Computational Design of Electrocatalysts for Sustainable Production of Synthetic Fuels
Department of Energy Conversion and Storage
Period: 01/09/2013 → 25/01/2017
Number of participants: 6
Phd Student:
Christensen, Rune (Intern)
Supervisor:
Hansen, Heine Anton (Intern)
Main Supervisor:
Vegge, Tejs (Intern)
Examiner:
Stephens, Ifan (Intern)
Reuter, Karsten (Ekstern)
Rossmeisl, Jan (Intern)

Financial sources
Source: Internal funding (public)
Name of research programme: Institut, samfinansiering

Relations
Publications:
Error Mitigation in Computational Design of Sustainable Energy Materials
Project: PhD

Design and testing of high performance regenerators
Department of Energy Conversion and Storage
Period: 15/08/2013 → 14/12/2016
Number of participants: 7
PhD Student:
Lei, Tian (Intern)
Supervisor:
Nielsen, Kaspar Kirstein (Intern)
Nielsen, Kaspar Kirstein (Intern)
Main Supervisor:
Engelbrecht, Kurt (Intern)
Examiner:
Hattel, Jesper Henri (Intern)
Barbosa Jr., Jader R. (Ekstern)
Furberg, Richard (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering

Relations
Publications:
Modeling of active magnetic regenerators and experimental investigation of passive regenerators with oscillating flow
Project: PhD

High performance Magnetocaloric Materials
Department of Energy Conversion and Storage
Period: 01/08/2013 → 30/09/2016
Number of participants: 7
PhD Student:
Neves Bez, Henrique (Intern)
Supervisor:
Nielsen, Kaspar Kirstein (Intern)
Smith, Anders (Intern)
Main Supervisor:
Bahl, Christian (Intern)
Examiner:
Bohr, Jakob (Intern)
Lo Bue, Martino (Ekstern)
Planes, Antoni (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering

Relations
Publications:
Magnetocaloric materials and first order phase transitions
Project: PhD

Computational Investigations of transport mechanisms across battery interfaces
Department of Energy Conversion and Storage
Period: 01/07/2013 → 16/11/2016
Number of participants: 6
PhD Student:
Loftager, Simon (Intern)
Supervisor:
Garcia-Lastra, Juan Maria (Ekstern)
Main Supervisor:
Vegge, Tejs (Intern)
Examiner:
Hjelm, Johan (Intern)
Khalifah, Peter (Ekstern)
Rossmeisl, Jan (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 FUU, 1/3 inst 1/3 Andet
Project: PhD

Exploring Electronic Properties in All-oxide Heterostructures
Department of Energy Conversion and Storage
Period: 01/07/2013 → 13/11/2017
Number of participants: 7
PhD Student:
Christensen, Dennis Valbjørn (Intern)
Supervisor:
Chen, Yunzhong (Intern)
Smith, Anders (Intern)
Main Supervisor:
Pryds, Nini (Intern)
Examiner:
Nygård, Jesper (Ekstern)
Eom, Chang-Beom (Intern)
Granozio, Fabio Miletto (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.
Project: PhD

Mixed Rare Earth-Fe-B sintered magnets
Department of Energy Conversion and Storage
Period: 15/06/2013 → 06/04/2017
Number of participants: 7
PhD Student:
Xia, Manlong (Intern)
Supervisor:
Abrahamsen, Asger Bech (Intern)
Pryds, Nini (Intern)
Main Supervisor:
Bahl, Christian (Intern)
Examiner:
Grivel, Jean-Claude (Intern)
Christensen, Mogens (Ekstern)
Paturi, Petriina (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Cost Effective Regenerative Metal Hydride Air Cell
Department of Energy Conversion and Storage
Atomic scale modelling and materials
Period: 01/06/2013 → 01/06/2014
Number of participants: 1
Metal Hydride Air Cell
Acronym: CERMAC
Project participant:
Blanchard, Didier (Intern)

Optimised Hybrid Magnets
Department of Energy Conversion and Storage
Period: 01/06/2013 → 16/11/2016
Number of participants: 7
Phd Student:
Insinga, Andrea Roberto (Intern)
Supervisor:
Bjørk, Rasmus (Intern)
Smith, Anders (Intern)
Main Supervisor:
Bahl, Christian (Intern)
Examiner:
Beleggia, Marco (Intern)
Jensen, Bogi Bech (Intern)
Lomonova, Elena A. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering

Relations
Publications:
Optimising Magnetostatic Assemblies
Project: PhD

Performance and lifetime limiting effects in Li-ion batteries
Department of Energy Conversion and Storage
Period: 01/06/2013 → 20/09/2016
Number of participants: 8
Phd Student:
Scipioni, Roberto (Intern)
Supervisor:
Hjelm, Johan (Intern)
Norby, Poul (Intern)
Main Supervisor:
Jensen, Søren Højgaard (Intern)
Examiner:
Bowen, Jacob R. (Intern)
Bowen, Jacob R. (Intern)
Lindbergh, Göran (Ekstern)
Lindbergh, Göran (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Offentlig finansiering

Relations
Publications:
Performance and Lifetime Limiting Effects in Li-ion Batteries
Project: PhD
Mobility and Interfacial Effects under Degradation of Polymer Solar Cells

Department of Energy Conversion and Storage
Period: 15/05/2013 → 16/06/2016
Number of participants: 6
Phd Student:
Corazza, Michael (Intern)
Supervisor:
Gevorgyan, Suren (Intern)
Main Supervisor:
Krebs, Frederik C (Intern)
Examiner:
Lauritzen, Hanne (Intern)
Kettle, Jeffrey Paul (Ekstern)
Maes, Wouter (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.

Relations
Publications:
Project: PhD

Materials for Energy Production

Department of Energy Conversion and Storage
Period: 01/05/2013 → 16/06/2016
Number of participants: 5
Phd Student:
Livi, Francesco (Intern)
Main Supervisor:
Bundgaard, Eva (Intern)
Examiner:
Lauritzen, Hanne (Intern)
Kettle, Jeffrey Paul (Ekstern)
Maes, Wouter (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Eksternt finansieret virksomhed

Relations
Publications:
Conjugated Polymers for Energy Production
Project: PhD

HT PEMFC Durability and Lifetime

Department of Energy Conversion and Storage
Period: 01/04/2013 → 24/01/2018
Number of participants: 7
Phd Student:
Søndergaard, Tonny (Intern)
Supervisor:
Cleemann, Lars Nielsenausen (Intern)
Li, Qingfeng (Intern)
Main Supervisor:
Jensen, Jens Oluf (Intern)
Examiner:
Petrushina, Irina (Intern)
Bajo, Justo Lobato (Ekstern)
Grahl-Madsen, Laila (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Offentlig finansiering
Project: PhD

**Mobility and Interfacial Effects under Degradation of Polymer Solar Cells**

Department of Energy Conversion and Storage
Period: 01/04/2013 → 16/06/2016
Number of participants: 5
Phd Student:
Roth, Bérenger (Intern)
Main Supervisor:
Krebs, Frederik C (Intern)
Examiner:
Lauritzen, Hanne (Intern)
Kettle, Jeffrey Paul (Ekstern)
Maes, Wouter (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.

Relations
Publications:
Operational stability of large scale OPV modules: interfaces, materials selection and stack design
Project: PhD

**Quantum and field effects of oxide heterostructures**

Department of Energy Conversion and Storage
Period: 01/03/2013 → 30/09/2016
Number of participants: 7
Phd Student:
Trier, Felix (Intern)
Supervisor:
Chen, Yunzhong (Intern)
Jesperersen, Thomas Sand (Ekstern)
Main Supervisor:
Pryds, Nini (Intern)
Examiner:
Thygesen, Kristian Sommer (Intern)
Gabay, Marc (Ekstern)
Granozio, Fabio Miletto (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut/centerfinansieret

Relations
Publications:
Quantum and field effects of oxide heterostructures
Project: PhD
**Powerpipe hybrid solar panel**

A solar collector panel both producing electricity and heat will be developed and tested.

Department of Civil Engineering

Section for Building Physics and Services

Department of Energy Conversion and Storage

PowerPipe ApS

Batec Solvarme A/S

LOKE Lolland Energi

Period: 01/01/2013 → 30/06/2014

Number of participants: 3

Solar collector, Hybrid, Electricity, Heat

Project participant:

Furbo, Simon (Intern)

Fan, Jianhua (Intern)

Perers, Bengt (Intern)

**Financing sources**

Source: Forskningsprojekter - Miljø- og Energinisteriet

Name of research programme: EUDP programme

Amount: 489,600.00 Danish Kroner

Year of approval: 2012

SMARTONICS FP7

The target of the Smartonics project is the development of Pilot lines that will combine smart technologies with smart nanomaterials for the precision synthesis of Organic Electronic (OE) devices

Department of Energy Conversion and Storage

Functional organic materials

Period: 01/01/2013 → 01/08/2014

Number of participants: 1

Project participant:

Beliatis, Michail (Intern)

**AC superconducting wires**


Department of Energy Conversion and Storage

Electrofunctional materials

Period: 01/01/2013 → 31/12/2013

Number of participants: 1

Superconductor, Coated conductor, Energy loss

Project participant:

Wulff, Anders Christian (Intern)

**In-situ Neutron Imaging of Solid Oxide Fuel Cells**

Department of Energy Conversion and Storage

Period: 01/01/2013 → 20/04/2016

Number of participants: 7

Phd Student:

Makowska, Małgorzata Grazyna (Intern)

Supervisor:
Investigation of performance and lifetime limiting effects in Li-air battery cells

Department of Energy Conversion and Storage
Period: 01/12/2012 → 22/02/2016
Number of participants: 6
PhD Student:
Knudsen, Kristian Bastholm (Intern)
Supervisor:
Jensen, Søren Højgaard (Intern)
Main Supervisor:
Hjelm, Johan (Intern)
Examiner:
Hagen, Anke (Intern)
Adelhelm, Philipp (Ekstern)
Edström, Ester Kristina (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 FUU, 1/3 inst 1/3 Andet
Project: PhD

Relations
Publications:
Alkali Metal-O₂ Batteries. Performance and Lifetime Limiting Effects
Project: PhD

Management of Lithium-air batteries - safety, reliability and performance

Department of Energy Conversion and Storage
Period: 01/12/2012 → 20/04/2016
Number of participants: 7
PhD Student:
Christensen, Andreas Elkjær (Intern)
Supervisor:
Larsen, Esben (Intern)
Vestin, Karl (Ekstern)
Main Supervisor:
Norby, Poul (Intern)
Examiner:
Jensen, Søren Højgaard (Intern)
Monroe, Charles William (Ekstern)
Møller, Per Jørgensen (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsstipendium
Project: PhD
Shaping our Energy Future with Electrospinning
Hans Christian Ørsted Postdoc Fellowship
Department of Energy Conversion and Storage
Ceramic Engineering & Science
Period: 15/10/2012 → 14/10/2014
Number of participants: 1
Project applicant:
Zhang, Wenjing (Angela) (Intern)

Oxygen Membranes for Biomass Gasification and Cement Industry
Department of Energy Conversion and Storage
Period: 01/09/2012 → 27/01/2016
Number of participants: 6
Phd Student:
Cheng, Shiyang (Intern)
Supervisor:
Kaiser, Andreas (Intern)
Main Supervisor:
Hendriksen, Peter Vang (Intern)
Examiner:
Kammer Hansen, Kent (Intern)
Guillon, Oliver (Ekstern)
Yu, Ji Haeng (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Preparation and characterization of cathode materials for lithium-oxygen batteries
Department of Energy Conversion and Storage
Period: 15/08/2012 → 20/09/2016
Number of participants: 6
Phd Student:
Storm, Mie Møller (Intern)
Supervisor:
Luntz, Alan (Ekstern)
Main Supervisor:
Norby, Poul (Intern)
Examiner:
Blanchard, Didier (Intern)
Choi, Jang Wook (Ekstern)
Nørgaard, Kasper (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering

Relations
Publications:
Preparation and Characterization of Cathode Materials for Lithium-Oxygen Batteries
Project: PhD

Towards Smart Grid Ready SOFC
Department of Energy Conversion and Storage
Applied Electrochemistry
IRD Fuel Cells A/S

Topsoe Fuel Cell
Period: 01/08/2012 → 31/07/2014
Number of participants: 1
solid oxide fuel cells , smart grid, reformate gas, electrochemistry, durability, load cycles, stacks
Project Coordinator:
Hjelm, Johan (Intern)
Project

Computational analysis and design of new materials for lithium-air batteries
Department of Energy Conversion and Storage
Period: 01/08/2012 → 02/12/2015
Number of participants: 7
Phd Student:
Mekonnen, Yedifana Setarge (Intern)
Supervisor:
Garcia-Lastra, Juan Maria (Ekstern)
Hummelshøj, Jens Strabo (Intern)
Main Supervisor:
Vegge, Tejs (Intern)
Examiner:
Blanchard, Didier (Intern)
Rossmeisl, Jan (Intern)
Siegel, Donald Jason (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Pressurized HT PEM Cells for H2/O2 operation
Department of Energy Conversion and Storage
Period: 01/08/2012 → 30/09/2015
Number of participants: 7
Phd Student:
Søndergaard, Stine (Intern)
Supervisor:
Cleemann, Lars Nilausen (Intern)
Jensen, Jens Oluf (Intern)
Main Supervisor:
Bjerrum, Niels J. (Intern)
Examiner:
Petrushina, Irina (Intern)
Schmidt, Thomas Justus (Ekstern)
Steenberg, Thomas (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut, samfinansiering
Project: PhD

Anion Conducting Polymer Membranes for Hydrogen Production Through Alkaline Water Electrolysis
Department of Energy Conversion and Storage
Proton conductors
Period: 01/07/2012 → 30/06/2014
Number of participants: 1
Acronym: AlkaPEM
Project participant:
Aili, David (Intern)

Miljøvenlige, organiske solceller med kontrolleret nanostruktur, baseret på partikler i vandig dispersion
Department of Energy Conversion and Storage
Period: 01/06/2012 → 30/09/2015
Number of participants: 6
PhD Student:
Pedersen, Emil Bøje Lind (Intern)
Supervisor:
Aanæs, Henrik (Intern)
Main Supervisor:
Andreasen, Jens Wenzel (Intern)
Examiner:
Poulsen, Henning Friis (Intern)
Müller, Christian (Ekstern)
Stingelin-Stutzmann, Natalie (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Hybrid metal-graphene nanostructured materials for innovative plasmonic electrodes
Department of Energy Conversion and Storage
Functional organic materials
Period: 01/03/2012 → 01/03/2014
Number of participants: 1
Acronym: UK EPSRC Postdoctoral Prize Fellowship
Project participant:
Beliatis, Michail (Intern)

Direct conversion of carbon to electricity in a hybrid solid oxide fuel cell
Department of Energy Conversion and Storage
Period: 01/03/2012 → 03/06/2015
Number of participants: 6
PhD Student:
Deleebeeck, Lisa (Intern)
Supervisor:
Mogensen, Mogens Bjerg (Intern)
Main Supervisor:
Kammer Hansen, Kent (Intern)
Examiner:
Hagen, Anke (Intern)
Lagergren, Carina (Ekstern)
Skou, Eivind Morten (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Anden EU-finansiering
Project: PhD
Electrolyte and electrocatalysts combinations suitable for CO2 reduction and O2 evolution

Department of Energy Conversion and Storage
Period: 01/03/2012 → 02/09/2015
Number of participants: 7
Phd Student:
Vico, Federica (Intern)
Supervisor:
Chatzichristodoulou, Christodoulos (Intern)
Holtappels, Peter (Intern)
Main Supervisor:
Mogensen, Mogens Bjerg (Intern)
Examiner:
Bonanos, Nikolaos (Intern)
Fabbri, Emiliana (Ekstern)
Sunde, Svein (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering

Relations
Publications:
Searching for electrolytes and electrodes for CO2 reduction below 300 °C
Project: PhD

Fabrication of Green Hydrocarbon Fuels via Capture and Electrolysis of CO2

Department of Energy Conversion and Storage
Period: 01/03/2012 → 13/05/2015
Number of participants: 7
Phd Student:
Ebbehøj, Søren Lyng (Intern)
Supervisor:
Jensen, Søren Højgaard (Intern)
Riisager, Anders (Intern)
Main Supervisor:
Mogensen, Mogens Bjerg (Intern)
Examiner:
Hendriksen, Peter Vang (Intern)
Hansen, John Begild (Ekstern)
Hartvigsen, Joseph J. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering

Relations
Publications:
Integration of CO2 air capture and solid oxide electrolysis for methane production
Project: PhD

Design and Optimization of Effective Segmented Thermoelectric Generator for Waste Heat Recovery

Department of Energy Conversion and Storage
Period: 01/02/2012 → 02/12/2015
Number of participants: 7
Phd Student:
Pham, Hoang Ngan (Intern)
A Novel Thermoelectric Power Generator
The overall aim of this project is to demonstrate a cost-effective, mass-producible, and environmentally friendly technology for producing a novel thermoelectric generator, which overcomes the drawbacks typically found in the conventional technology. This type of thermal-to-electrical generating technology has broad applications ranging from a few mW up to kW devices. In order to achieve this goal, a thermoelectric module using an inexpensive ceramic forming process (tape casting) will be made during this project.

Thermo Ceramics
Electrofunctional materials

Development of novel electrode-catalyst materials for Li-air battery cathodes
Department of Energy Conversion and Storage
Period: 01/01/2012 → 01/07/2015
Number of participants: 7
PhD Student:
Højberg, Jonathan (Intern)
Supervisor:
Johansen, Keld (Ekstern)
Main Supervisor:
Vege, Tejs (Intern)
Examiner:
García Lastra, Juan Maria (Intern)
Edström, Ester Kristina (Ekstern)
Hoster, Harry Ernst (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsstipendium
Project: PhD

High-efficiency, low-cost electrode surfaces for next generation alkaline electrolysis
Department of Energy Conversion and Storage
Proton conductors
Energy and Materials
Hydrogen from RES: pressurised alkaline electrolyser with high efficiency

The project RESelyser develops high pressure, highly efficient, low cost alkaline water electrolysers that can be integrated with renewable energy power sources (RES) using an advanced membrane concept, highly efficient electrodes and a new cell concept. A new concept with a three electrolyte loop system will be developed demonstrating even higher performance than conventional two electrolyte loop systems. This three electrolyte loop system will use a new separator membrane with internal electrolyte circulation and an adapted cell to improve mass transfer, especially gas evacuation. Intermittent and varying load operation connected to an RES will be addressed by improved electrode stability and a cell concept for increasing the gas purity of hydrogen and oxygen especially at low power as well as by a system concept. Electrolysers up to 30 kW with 6 Nm³/h hydrogen production will be realized in the project. The primary pressure of the electrolysers will be above 25 bar (without the use of a compressor) to reduce the power loss for hydrogen compression to a minimum. All components of the system will be analyzed for their costs and developed to reduce the system price such that hydrogen can be produced at 3000 €/(Nm³/h). An extrapolation to a primary electrolysers pressure of 100-150 bar is considered.
Project

**Solar Hydrogen Fuel Production Station**

Department of Energy Conversion and Storage

Functional organic materials  
Period: 31/10/2011 → 01/09/2012  
Number of participants: 1  
Acronym: UK Knowledge Transfer Account (KTA)  
Project participant:  
Beliatis, Michail (Intern)

**Kinetic studies and Computational Fluid Dynamics (CFD) simulations to aid in the development of Tantalum coated extreme corrosion resistance welded plate heat exchangers (ECWP)**

Department of Energy Conversion and Storage  
Period: 01/10/2011 → 17/12/2014  
Number of participants: 8  
PhD Student:  
Mugabi, James Atwoki (Intern)  
Supervisor:  
Christensen, Erik (Intern)  
Eriksen, Søren (Intern)  
Petrushina, Irina (Intern)  
Main Supervisor:  
Bjerrum, Niels J. (Intern)  
Examiner:  
Li, Qingfeng (Intern)  
Papatheodorou, George (Ekstern)  
Skou, Eivind Morten (Ekstern)

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Institut stipendie (DTU) Samf.  
Project: PhD

**Modelling environmentally friendly materials for magnetic refrigeration**

Department of Energy Conversion and Storage  
Period: 01/10/2011 → 17/12/2014  
Number of participants: 7  
PhD Student:  
von Moos, Lars (Intern)  
Supervisor:  
Engelbrecht, Kurt (Intern)  
Nielsen, Kaspar Kirstein (Intern)  
Main Supervisor:  
Bahl, Christian (Intern)  
Examiner:  
Abrahamsen, Asger Bech (Intern)  
Burriel, Ramón (Ekstern)  
Cohen, Lesley (Ekstern)

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Institut, samfinansiering  
Project: PhD
Computational Design of New Materials for Ammonia Storage

Department of Energy Conversion and Storage
Period: 15/09/2011 → 17/12/2014
Number of participants: 6
Phd Student: Jensen, Peter Bjerre (Intern)
Supervisor: Quaade, Ulrich (Intern)
Main Supervisor: Vegge, Tejs (Intern)
Examiner: Rossmeisl, Jan (Intern)
Bligaard, Thomas (Intern)
Hammer, Bjørk (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 FUU, 1/3 inst 1/3 Andet
Project: PhD

Fremstilling og karakterisering af elektrolytter og elektroder til vandelektrolyse i temperaturområdet 200-400C

Department of Energy Conversion and Storage
Period: 15/09/2011 → 11/03/2015
Number of participants: 8
Phd Student: Prag, Carsten Brorson (Intern)
Supervisor: Christensen, Erik (Intern)
Petrushina, Irina (Intern)
Li, Qingfeng (Intern)
Main Supervisor: Bjerrum, Niels J. (Intern)
Examiner: Berg, Rolf W. (Intern)
Steenberg, Thomas (Intern)
Sunde, Svein (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.
Project: PhD

Fremstilling og karakterisering daf materiale og komponenter til mellemliggende emperatur brændselsceller og vandelektrolyse

Department of Energy Conversion and Storage
Period: 15/08/2011 → 26/11/2014
Number of participants: 8
Phd Student: Jensen, Annemette Hindhede (Intern)
Supervisor: Barner, Jens H. Von (Intern)
Christensen, Erik (Intern)
Li, Qingfeng (Intern)
Main Supervisor: Bjerrum, Niels J. (Intern)
Examiner: Petrushina, Irina (Intern)
**Development and processing of p-type oxide thermoelectric materials**

Department of Energy Conversion and Storage  
Period: 01/08/2011 → 26/11/2014  
Number of participants: 7  
PhD Student:  
Wu, NingYu (Intern)  
Supervisor:  
Nong, Ngo Van (Ekstern)  
Pryds, Nini (Intern)  
Main Supervisor:  
Linderoth, Søren (Intern)  
Examiner:  
Bahl, Christian (Intern)  
Balke, Benjamin (Ekstern)  
Eklund, Per (Ekstern)  

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Institut stipendie (DTU) Samf.  
Project: PhD

**Modeling of shape instabilities occurring during sintering**

Department of Energy Conversion and Storage  
Period: 15/07/2011 → 30/09/2014  
Number of participants: 7  
PhD Student:  
Tadesse Molla, Tesfaye (Intern)  
Supervisor:  
Bjørk, Rasmus (Intern)  
Pryds, Nini (Intern)  
Main Supervisor:  
Frandsen, Henrik Lund (Intern)  
Examiner:  
Hattel, Jesper Henri (Intern)  
Bordia, Rajendra K. (Ekstern)  
Raether, Friedrich (Ekstern)  

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Forskningsrådsfinsiering  
Project: PhD

**Development and processing of n-type oxide thermoelectric materials**

Department of Energy Conversion and Storage  
Period: 01/07/2011 → 30/09/2014  
Number of participants: 7  
PhD Student:  
Han, Li (Intern)  
Supervisor:
Development of functionally graded thermoelectric materials based on optimal average figure-of-merit

Department of Energy Conversion and Storage
Period: 01/06/2011 → 26/11/2014
Number of participants: 5
Phd Student:
Le, Thanh Hung (Intern)
Main Supervisor:
Pryds, Nini (Intern)
Examiner:
Kuhn, Luise Theil (Intern)
Gelbstein, Yaniv (Ekstern)
Rosendahl, Lasse (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Experimental tape casting of multilayer for flue gas purification

Department of Energy Conversion and Storage
Period: 15/05/2011 → 30/09/2015
Number of participants: 7
Phd Student:
Schmidt, Cristine Grings (Intern)
Supervisor:
Andersen, Kjeld Bøhm (Intern)
Kammer Hansen, Kent (Intern)
Main Supervisor:
Kaiser, Andreas (Intern)
Examiner:
Chatzichristodoulou, Christodoulos (Intern)
Graule, Thomas J. (Ekstern)
Görmann, Claus Friedrich (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Experimental Extrusion of Tubular Multilayer Materials for Oxygen Membranes

Department of Energy Conversion and Storage
Period: 01/05/2011 → 17/12/2014
Number of participants: 8
Inorganic Proton Conducting Materials
Department of Energy Conversion and Storage
Period: 15/04/2011 → 24/09/2014
Number of participants: 6
Phd Student: Anfimova, Tatiana (Intern)
Supervisor: Bjerrum, Niels J. (Intern)
Main Supervisor: Li, Qingfeng (Intern)
Examiner: Bonanos, Nikolaos (Intern)
Jensen, Torben René (Intern)
Norby, Truls (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.
Project: PhD

Experimental Tape Casting of Adjacently Graded Materials for Magnetic Refrigeration
Department of Energy Conversion and Storage
Period: 01/04/2011 → 26/11/2014
Number of participants: 8
Phd Student: Bulatova, Regina (Intern)
Supervisor: Andersen, Kjeld Bøhm (Intern)
Della Negra, Michela (Intern)
Kaiser, Andreas (Intern)
Main Supervisor: Bahl, Christian (Intern)
Examiner: Agersted, Karsten (Ekstern)
Ringgaard, Erling (Intern)
Roosen, Andreas (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
SOFC Stack Diagnostics

Department of Energy Conversion and Storage
Period: 01/04/2011 → 04/02/2015
Number of participants: 7
Phd Student:
Mosbæk, Rasmus Rode (Intern)
Supervisor:
Barfod, Rasmus Gottrup (Intern)
Hendriksen, Peter Vang (Intern)
Main Supervisor:
Hjelm, Johan (Intern)
Examiner:
Nielsen, Jimmi (Intern)
Haart, L. G. J. de (Ekstern)
Weber, André (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut, samfinansiering
Project: PhD

Adiabatic Liquid Piston Compressed Air Energy Storage
Traditional Compressed Air Energy Storage (CAES) is seen as one of the most cost effective technologies for the bulk energy storage in the future flexible grid. The project will investigate the possible lift of the round trip efficiency by the introduction of Adiabatic Liquid Piston CAES (ALP-CAES) which is expected to be highly competitive.

Department of Mechanical Engineering
Energy Engineering
Thermal Energy
Risø National Laboratory for Sustainable Energy
Secretariat, IT
Department of Energy Conversion and Storage
Materials Research Division
Nano-Microstructures in Materials
Administration Department
Functional organic materials
Period: 01/03/2011 → ...
Number of participants: 6
Acronym: ALP-CAES
Project participant:
Bang-Møller, Christian (Intern)
Elmegaard, Brian (Intern)
Pedersen, Allan Schröder (Intern)
Pedersen, Aksel Hauge (Ekstern)
Crotogino, Fritz (Ekstern)
Project Manager, academic:
Reinholdt, Lars (Ekstern)

Medium Temperature Water Electrolysis
Hydrogen has the potential to provide a reliable, secure and clean source of power. Water offers a practical way of hydrogen production in association with renewable energy sources. The main challenges for water electrolyzers are high cost, low efficiency and insufficient lifetime. The strategy of MEDLYS to address these issues is to develop novel materials
and technologies for a medium temperature steam electrolyser operating at 200-400°C. The temperature range is optimal for 1) improving thermodynamics and kinetics of the process, 2) potentially replacing noble metal based catalysts with cost-effective alternatives, 3) allowing for a wide selection of construction materials from metals, ceramics and thermal plastics for conducting, insulating or sealing purposes and 4) maintaining long-term durability. MEDLYS will start with development of fundamental materials including inorganic/composite proton conducting electrolyte, alternative catalysts and other construction (electrode substrate, current collector, and bipolar plate) materials. Based on the materials, electrolyser components will be manufactured and a lab-scale cell will be constructed for evaluation and concept-proof test. The proposal is based on the results from ongoing activities within DSF HyCycle Center by most of the consortium partners, who have expertise from materials science and technological know-how and strong intention to further exploit the achievements after the project. The fulfilment of MEDLYS objectives is believed to bring breakthroughs in the hydrogen production technology, which, in turn, would promote the renewable energy technologies on a national as well as an European and global level.

Department of Energy Conversion and Storage
Proton conductors
Energy and Materials
Department of Chemistry
Department of Physics
Experimental Surface and Nanomaterials Physics
University of Southern Denmark
Technical University of Munich
Danish Power Systems ApS
Tantaline A/S
Period: 01/03/2011 → 28/02/2015
Number of participants: 6
Acronym: MEDLYS
Number of related Ph.D. students: 1
Project participant:
Christensen, Erik (Intern)
Barner, Jens H. Von (Intern)
Li, Qingfeng (Intern)
Chorkendorff, Ib (Intern)
Petrushina, Irina (Intern)
Project Coordinator:
Bjerrum, Niels J. (Intern)
Project

Udvikling og karakterisering af avancerede Li-batterier
Department of Energy Conversion and Storage
Period: 01/03/2011 → 02/09/2015
Number of participants: 7
Phd Student:
Christiansen, Ane Sæland (Intern)
Supervisor:
Jensen, Søren Højgaard (Intern)
Norby, Poul (Intern)
Main Supervisor:
Holtappels, Peter (Intern)
Examiner:
Pedersen, Allan Schrøder (Intern)
Dahl, Søren (Intern)
Dominko, Robert (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut, samfinansiering
In situ characterisation of structure and transport in battery electrolytes and electrodes

Department of Energy Conversion and Storage
Period: 01/01/2011 → 26/02/2014
Number of participants: 7
Phd Student:
Sveinbjörnsson, Dadi Þorsteinn (Intern)
Supervisor:
Mogensen, Mogens Bjerg (Intern)
Norby, Poul (Intern)
Main Supervisor:
Vegge, Tejs (Intern)
Examiner:
Hjelm, Johan (Intern)
David, William Ian Fraser (Ekstern)
Sørby, Magnus H. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Globaliseringsmidler
Project: PhD

Polymer photovoltaics - Largecells - R2R-produced polymer solar cells

Department of Energy Conversion and Storage
Period: 01/01/2011 → 26/02/2014
Number of participants: 5
Phd Student:
Hösel, Markus (Intern)
Main Supervisor:
Krebs, Frederik C (Intern)
Examiner:
Andreasen, Jens Wenzel (Intern)
Laursen, Bo Wegge (Intern)
Lianos, Panagiotis (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Anden EU-finansiering
Project: PhD

Investigation of the degradation of solid oxide cells applied for electrolysis

Department of Energy Conversion and Storage
Period: 15/12/2010 → 26/02/2014
Number of participants: 6
Phd Student:
Tao, Youkun (Intern)
Supervisor:
Ebbesen, Sune Dalgaard (Intern)
Main Supervisor:
Mogensen, Mogens Bjerg (Intern)
Examiner:
Nielsen, Jimmi (Intern)
Brisse, Annabelle (Ekstern)
Irvine, John T. S. (Ekstern)

Financing sources
Use of Biomass derived fuels for SOFC’s effect of fuel impurities

Department of Energy Conversion and Storage
Period: 15/12/2010 → 15/04/2016
Number of participants: 3
Phd Student:
Johnson, Gregory (Intern)
Supervisor:
Hjalmarsson, Per (Intern)
Main Supervisor:
Hagen, Anke (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

OXIDE THERMOELECTRICS FOR EFFECTIVE POWER GENERATION FROM WASTE HEAT

Department of Energy Conversion and Storage
Electrofunctional materials
Period: 01/12/2010 → …
Number of participants: 1
Acronym: OTE-POWER
Project Manager, academic:
Van Nong, Ngo (Intern)

Financing sources
Source: Public research council
Name of research programme: The Danish Council for Strategic Research DSF
Amount: 21,000,000.00 Danish Kroner

Risk-benefit analyser af funktionelle fødevarer – Fokus på D-vitamin

National Food Institute
Division of Food Chemistry
Division of Toxicology and Risk Assessment
Department of Energy Conversion and Storage
Mixed Conductors
Period: 01/12/2010 → 30/11/2014
Number of participants: 4
Project participant:
Burild, Anders (Intern)
Poulsen, Morten (Intern)
Frandsen, Henrik Lund (Intern)
Project Manager, organisational:
Jakobsen, Jette (Intern)

Degradation of nanoparticle composite solar cells comprising both organic and inorganic materials

Department of Energy Conversion and Storage
Period: 01/10/2010 → 13/05/2015
Number of participants: 6
Phd Student:
Andreasen, Birgitta (Intern)
Supervisor:
Krebs, Frederik C (Intern)
Main Supervisor:
Norman, Kion (Intern)
Examiner:
Kuhn, Luise Theil (Intern)
A. Katz, Eugene (Ekstern)
Persson, Nils-Krister (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Grundforskningsfonden
Project: PhD

Nano-Structures of Organic-based photovoltaic Cells
Department of Energy Conversion and Storage
Period: 01/10/2010 → 18/12/2013
Number of participants: 7
Phd Student:
Böttiger, Arvid P.L. (Intern)
Supervisor:
Krebs, Frederik C (Intern)
Yang, Xiaoni (Ekstern)
Main Supervisor:
Andreasen, Jens Wenzel (Intern)
Examiner:
Bahl, Christian (Intern)
Moth-Poulsen, Kasper (Intern)
Persson, Nils-Krister (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Grundforskningsfonden
Project: PhD

Organic-based photovoltaic cells with morphology control
Department of Energy Conversion and Storage
Period: 01/10/2010 → 11/12/2013
Number of participants: 6
Phd Student:
Andersen, Thomas Rieks (Intern)
Supervisor:
Jørgensen, Mikkel (Intern)
Main Supervisor:
Bundgaard, Eva (Intern)
Examiner:
Kuhn, Luise Theil (Intern)
Brabec, Christoph J. (Ekstern)
Lira-Cantu, Mónica (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Grundforskningsfonden
Project: PhD
Roll-to-roll adaptation of high efficiency organic-based photovoltaic cells

Department of Energy Conversion and Storage
Period: 01/10/2010 → 24/09/2014
Number of participants: 5
Phd Student:
Trofod, Thue (Intern)
Main Supervisor:
Krebs, Frederik C (Intern)
Examiner:
Holtappels, Peter (Intern)
Moons, Ellen (Ekstern)
Thompson, Barry C. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Grundforskningsfonden
Project: PhD

Large-area Organic and Hybrid Solar Cells

Department of Energy Conversion and Storage
Functional organic materials
Period: 01/09/2010 → 31/08/2014
Number of participants: 2
Acronym: Largecells
Project participant:
Krebs, Frederik C (Intern)
Søndergaard, Roar R. (Intern)

Relations
Publications:
Reversible degradation of inverted organic solar cells by concentrated sunlight
The use of polyurethane as encapsulating method for polymer solar cells—An inter laboratory study on outdoor stability in 8 countries
Interlaboratory outdoor stability studies of flexible roll-to-roll coated organic photovoltaic modules: Stability over 10,000 h
Roll-to-roll fabrication of polymer solar cells
Electrical and Photo-Induced Degradation of ZnO Layers in Organic Photovoltaics
Origin of size effect on efficiency of organic photovoltaics
Scalability and stability of very thin roll-to-roll processed large area indium-tin-oxide free polymer solar cell modules
The OE-A OPV demonstrator anno domini 2011
Solar cells with one-day energy payback for the factories of the future
Large-scale roll-to-roll photonic sintering of flexo printed silver nanoparticle electrodes
The ISOS-3 inter-laboratory collaboration focused on the stability of a variety of organic photovoltaic devices
Investigation of the degradation mechanisms of a variety of organic photovoltaic devices by combination of imaging techniques—the ISOS-3 inter-laboratory collaboration
Rapid flash annealing of thermally reactive copolymers in a roll-to-roll process for polymer solar cells
TOF-SIMS investigation of degradation pathways occurring in a variety of organic photovoltaic devices – the ISOS-3 inter-laboratory collaboration
Roll-to-Roll fabrication of large area functional organic materials
Polymer and organic solar cells viewed as thin film technologies: What it will take for them to become a success outside academia
On the stability of a variety of organic photovoltaic devices by IPCE and in situ IPCE analyses – the ISOS-3 inter-laboratory collaboration
Enhancing functionality of ZnO hole blocking layer in organic photovoltaics
Comparison of UV-Curing, Hotmelt, and Pressure Sensitive Adhesive as Roll-to-Roll Encapsulation Methods for Polymer Solar Cells
All solution processing of ITO-free organic solar cell modules directly on barrier foil
A rational method for developing and testing stable flexible indium- and vacuum-free multilayer tandem polymer solar cells comprising up to twelve roll processed layers
Economic assessment of solar electricity production from organic-based photovoltaic modules in a domestic environment
Stability of Polymer Solar Cells
Slot-die Coating of a High Performance Copolymer in a Readily Scalable Roll Process for Polymer Solar Cells
Comparison of Fast Roll-to-Roll Flexographic, Inkjet, Flatbed, and Rotary Screen Printing of Metal Back Electrodes for Polymer Solar Cells

New types of electrocatalysts for electrolysis and fuel cells
Department of Energy Conversion and Storage
Period: 01/09/2010 → 03/02/2014
Number of participants: 7
PhD Student:
Tomás García, Antonio Luis (Intern)
Supervisor:
Petrushina, Irina (Intern)
Li, Qingfeng (Intern)
Main Supervisor:
Bjerrum, Niels J. (Intern)
Examiner:
Berg, Rolf W. (Intern)
Shen, Pei Kang (Ekstern)
Skou, Eivind Morten (Ekstern)

Financial sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.
Project: PhD

Theoretical investigations of novel materials for nitrogen fixation
Department of Energy Conversion and Storage
Period: 01/09/2010 → 11/12/2013
Number of participants: 6
PhD Student:
Howalt, Jakob Geelmuyden (Intern)
Supervisor:
Bligaard, Thomas (Intern)
Main Supervisor:
Vegge, Tejs (Intern)
Examiner:
Holtappels, Peter (Intern)
Hammer, Bjørk (Intern)
Hellman, Anders (Ekstern)

Financial sources
Source: Internal funding (public)
Name of research programme: 1/3 FUU, 1/3 inst 1/3 Andet
Project: PhD

Upscaling of Highly Flexible Polymer Solar Cells
Department of Energy Conversion and Storage
Period: 01/09/2010 → 26/02/2014
Number of participants: 5
PhD Student:
Angmo, Dechan (Intern)
Main Supervisor:
Krebs, Frederik C (Intern)
Examiner:
Holtappels, Peter (Intern)
Moons, Ellen (Ekstern)
Thompson, Barry C. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Danish-Chinese Center for Organic based Photovoltaic Cells with Morphology Control
Department of Energy Conversion and Storage

Functional organic materials
Imaging and Structural Analysis
Period: 31/08/2010 → 31/08/2016
Number of participants: 12
Number of related Ph.D. students: 1
Project participant:
Oksbjerg, Birgit (Intern)
Trofod, Thue (Intern)
Bundgaard, Eva (Intern)
Andreasen, Jens Wenzel (Intern)
Norman, Kion (Intern)
Krebs, Frederik C (Intern)
Zawacka, Natalia Klaudia (Intern)
Jørgensen, Mikkel (Intern)
Angmo, Dechan (Intern)
Andersen, Thomas Rieks (Intern)
Bentzen, Janet Jonna (Intern)
Rossander, Lea Hildebrandt (Intern)

Relations
Activities:
High resolution ptychographic tomography of soft matter
Publications:
Spatial degradation mapping and componentwise degradation tracking in polymer-fullerene blends
Scalable, ambient atmosphere roll-to-roll manufacture of encapsulated large area, flexible organic tandem solar cell modules
In situ monitoring of structure formation in the active layer of polymer solar cells during roll-to-roll coating
The influence of additives on the morphology and stability of roll-to-roll processed polymer solar cells studied through ex situ and in situ X-ray scattering
Enabling Flexible Polymer Tandem Solar Cells by 3D Ptychographic Imaging
All-Solution-Processed, Ambient Method for ITO-Free, Roll-Coated Tandem Polymer Solar Cells using Solution-Processed Metal Films
Medium area, flexible single and tandem junction solar cells based on roll coated semi-random copolymers
Roll-coating fabrication of flexible large area small molecule solar cells with power conversion efficiency exceeding 1%
Comparison of additive amount used in spin-coated and roll-coated organic solar cells

Højtemperatur PEM Brandselsceller og organiske brændsler
Department of Energy Conversion and Storage
**Indium-tin-oxide free roll-to-roll processed polymer solar cells**

Department of Energy Conversion and Storage

Period: 01/08/2010 → 11/12/2013
Number of participants: 5
Phd Student: Dam, Henrik Friis (Intern)
Main Supervisor: Krebs, Frederik C (Intern)
Examiner: Brabec, Christoph J. (Ekstern)
Kuhn, Luise Theil (Intern)
Yu, Donghong (Ekstern)

**Financing sources**

Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

**Large Area Roll-to-roll processed photocatalytic films for solar energy conversion and storage**

Department of Energy Conversion and Storage

Period: 01/08/2010 → 26/02/2014
Number of participants: 5
Phd Student: Jensen, Jacob (Intern)
Main Supervisor: Krebs, Frederik C (Intern)
Examiner: Andreasen, Jens Wenzel (Intern)
Laursen, Bo Wegge (Intern)
Lianos, Panagiotis (Ekstern)

**Financing sources**

Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

**Development and application of a green Chemistry solution deposition technique for buffer layer coating on cue-textured metal substrates in view of further deposition of rare-earth based superconductors**

Department of Energy Conversion and Storage
Development of a fluorine-free chemical solution deposition route for rare-earth cuprate superconducting tapes and its application to reel-to-reel

Department of Energy Conversion and Storage
Period: 01/07/2010 → 30/09/2013
Number of participants: 5
Phd Student: Tang, Xiao (Intern)
Main Supervisor: Grivel, Jean-Claude (Intern)
Examiner: Agersted, Karsten (Ekstern)
Augieri, Andrea (Ekstern)
Driessche, Isabel J. M. Van (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Durable and Robust SOFC
This 2-year project had as one of its’ overarching goals to improve durability and robustness of the Danish solid oxide fuel cells. The project focus was on cells and cell components suitable for SOFC operation in the temperature range 600 – 750 °C. The cells developed and/or studied in this project are intended for use within the CHP (Combined Heat and Power) market segment with stationary power plants in the range 1 – 250 kW e in mind. A significant part of this project was concerned with improved understanding of degradation and failure mechanisms.

Department of Energy Conversion and Storage
Applied Electrochemistry
IRD Fuel Cells A/S
Period: 01/07/2010 → 30/06/2012
Number of participants: 1

solid oxide fuel cells, electrochemistry, degradation, durability, lifetime limiting factors, porous electrode, functional ceramics, high temperature materials, hydrogen
Project Coordinator: Hjelm, Johan (Intern)

Financing sources
Source: Public research programme (public)
Name of research programme: ForskEL (Energinet.dk)
Web address: http://www.forskel.dk
Amount: 11,000,000.00 Danish Kroner
Year of approval: 2010
Project
Electrolytes for electrochemical N2 fixation cells

Department of Energy Conversion and Storage
Period: 15/05/2010 → 30/09/2013
Number of participants: 6
Phd Student:
Lapina, Alberto (Intern)
Supervisor:
Mogensen, Mogens Bjerg (Intern)
Main Supervisor:
Holtappels, Peter (Intern)
Examiner:
Vegge, Tejs (Intern)
Haart, L. G. J. de (Ekstern)
Irvine, John T. S. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 DTU-stip, 2/3 FUR/andet
Project: PhD

Low Temperature oxidation of hydrocarbons using an electrochemical reactor

Department of Energy Conversion and Storage
Period: 01/05/2010 → 19/08/2013
Number of participants: 6
Phd Student:
Ippolito, Davide (Intern)
Supervisor:
Christensen, Henrik (Ekstern)
Main Supervisor:
Kammer Hansen, Kent (Intern)
Examiner:
Bonanos, Nikolaos (Intern)
Marnellos, George E. (Ekstern)
Skou, Eivind Morten (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Degradation mechanism of the LSCF Cathode

Department of Energy Conversion and Storage
Period: 15/04/2010 → 19/03/2013
Number of participants: 7
Phd Student:
Zhang, Weiwei (Intern)
Supervisor:
Barfod, Rasmus Gottrup (Intern)
Hendriksen, Peter Vang (Intern)
Main Supervisor:
Chen, Ming (Intern)
Examiner:
Hjelm, Johan (Intern)
Hallstedt, Bengt (Ekstern)
Markus, Torsten (Ekstern)
Financing sources
Source: Internal funding (public)
Name of research programme: DTU, Samfinansiering
Project: PhD

Development of improved electrodes in high temperature PEM fuel cells
Department of Energy Conversion and Storage
Period: 15/03/2010 → 11/12/2013
Number of participants: 7
Phd Student:
Permyakova, Anastasia Aleksandrovna (Intern)
Supervisor:
Jensen, Jens Oluf (Intern)
Li, Qingfeng (Intern)
Main Supervisor:
Bjerrum, Niels J. (Intern)
Examiner:
Christensen, Erik (Intern)
Arenz, Matthias (Ekstern)
Bajo, Justo Lobato (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU, Samfinansiering
Project: PhD

BioSOFC - 3rd Generation Biomass Based Combined Heat and Power (CHP)
The aim of project is to investigate the combination of biomass gasification with SOFC in an efficient decentralized and flexible energy system for small scale combined heat and power production. The project work includes design, construction and long term operation of a gasifier-SOFC stack test set-up, analysis of performance and system analysis.

Department of Mechanical Engineering
Energy Engineering
Thermal Energy
Risø National Laboratory for Sustainable Energy
Department of Chemical and Biochemical Engineering
Biosystems Division
CHEC Research Centre
Biomass Gasification
Department of Energy Conversion and Storage
Fuel Cells and Solid State Chemistry Division
Applied Electrochemistry
Electrochemical Evaluation
Period: 01/03/2010 → 01/03/2013
Number of participants: 7
Acronym: BioSOFC
Project participant:
Bang-Møller, Christian (Intern)
Ahrenfeldt, Jesper (Intern)
Elmegaard, Brian (Intern)
Rokni, Masoud (Intern)
Hagen, Anke (Intern)
Hansen, John Bøgild (Ekstern)
Low Temperature NOx decomposition using an electrochemical Reactor

Department of Energy Conversion and Storage
Period: 01/03/2010 → 19/08/2013
Number of participants: 5
Phd Student:
Shao, Jing (Intern)
Main Supervisor:
Kammer Hansen, Kent (Intern)
Examiner:
Hjelm, Johan (Intern)
Kustov, Arkadii (Intern)
Vernoux, Philippe (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Test and Approval Center for Fuel Cell and Hydrogen Technologies: Phase I. Initiation

Department of Energy Conversion and Storage
Applied Electrochemistry
Danish Gas Technology Centre A/S
Period: 01/01/2010 → 30/06/2012
Number of participants: 1
Project participant:
Hagen, Anke (Intern)

Relations
Publications:
Accelerated testing of solid oxide fuel cell stacks for micro combined heat and power application

Electrolytes for Synthesis of CO2-neutral Fuels

Department of Energy Conversion and Storage
Period: 01/01/2010 → 19/08/2013
Number of participants: 7
Phd Student:
Hallinder, Jonathan (Intern)
Supervisor:
Hagen, Anke (Intern)
Mogensen, Mogens Bjerg (Intern)
Main Supervisor:
Holtappels, Peter (Intern)
Examiner:
Li, Qingfeng (Intern)
Grahl-Madsen, Laila (Ekstern)
Stimming, Ulrich (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 DTU-stip, 2/3 FUR/andet
Project: PhD
Electrochemical Removal of NOx and Hydrocarbons

Department of Energy Conversion and Storage
Period: 01/12/2009 → 17/12/2014
Number of participants: 5
Phd Student:
Friedberg, Anja Zarah (Intern)
Main Supervisor:
Kammer Hansen, Kent (Intern)
Examiner:
Jensen, Søren Højgaard (Intern)
Rasmussen, Søren Birk (Intern)
Tsiplakides, Dimitrios T. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Synthesis of new polymer materials for high efficiency photovoltaire cells

Department of Energy Conversion and Storage
Period: 01/10/2009 → 24/06/2013
Number of participants: 6
Phd Student:
Carlé, Jon Eggert (Intern)
Supervisor:
Krebs, Frederik C (Intern)
Main Supervisor:
Jørgensen, Mikkel (Intern)
Examiner:
Sommer-Larsen, Peter (Intern)
Christensen, Jørn B. (Ekstern)
R. Andersson, Mats (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Computational analysis of the interaction of water with materials for energy storage

Department of Energy Conversion and Storage
Period: 15/09/2009 → 19/03/2013
Number of participants: 6
Phd Student:
Lysgaard, Steen (Intern)
Supervisor:
Bligaard, Thomas (Intern)
Main Supervisor:
Vegge, Tejs (Intern)
Examiner:
Rossmeisl, Jan (Intern)
Hellman, Anders (Ekstern)
Jónsson, Hannes (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD
Computational screening of new carbon-neutral energy materials
Department of Energy Conversion and Storage
Period: 15/09/2009 → 19/03/2013
Number of participants: 6
Phd Student:
Mýrdal, Jón Steinar Garðarsson (Intern)
Supervisor:
Rossmeisl, Jan (Intern)
Main Supervisor:
Vegge, Tejs (Intern)
Examiner:
Schiatz, Jakob (Intern)
David, William Ian Fraser (Ekstern)
Ikeshoji, Tamio (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 DTU-stip, 2/3 FUR/andet
Project: PhD

Development of long cube textured metal substrates suitable for reel-to-reel processing and applications under both ac and dc conditions
Department of Energy Conversion and Storage
Period: 01/09/2009 → 28/01/2013
Number of participants: 7
Phd Student:
Wulff, Anders Christian (Intern)
Supervisor:
Andersen, Niels Hessel (Intern)
Mishin, Oleg (Intern)
Main Supervisor:
Grivel, Jean-Claude (Intern)
Examiner:
Juul Jensen, Dorte (Intern)
Glowacki, Bartek A. (Ekstern)
Holzapfel, Bernhard (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Nanostructured Ceramic Oxygen Sensors
Department of Energy Conversion and Storage
Period: 01/09/2009 → 17/12/2012
Number of participants: 6
Phd Student:
Hu, Qiang (Intern)
Supervisor:
Hansen, Karin Vels (Intern)
Main Supervisor:
Mogensen, Mogens Bjerg (Intern)
Examiner:
Holtappels, Peter (Intern)
Skou, Eivind Morten (Ekstern)
Wiemhöfer, Hans-Dieter (Ekstern)
Financing sources
Source: Internal funding (public)
Name of research programme: Offentlig finansiering
Project: PhD

New Electrolytes for CO2 Electrolysis Cells
Department of Energy Conversion and Storage
Period: 01/09/2009 → 19/03/2013
Number of participants: 7
Phd Student:
Mollerup, Pia Lolk (Intern)
Supervisor:
Bonanos, Nikolaos (Intern)
Tullmar, Peter Blennov (Ekstern)
Main Supervisor:
Holtappels, Peter (Intern)
Examiner:
Jensen, Jens Oluf (Intern)
Friedrich, Kaspar Andreas (Ekstern)
Kiros, Yohannes (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Lengthening the Lifetime of R2R-produced Polymer Solar Cells
Department of Energy Conversion and Storage
Period: 01/08/2009 → 24/06/2013
Number of participants: 5
Phd Student:
Madsen, Morten Vesterager (Intern)
Supervisor:
Krebs, Frederik C (Intern)
Main Supervisor:
Norrman, Kion (Intern)
Examiner:
Kuhn, Luise Theil (Intern)
A. Katz, Eugene (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Programbevilling
Project: PhD

High Performance polymer solar cells through rational characterization and design
Department of Energy Conversion and Storage
Period: 01/07/2009 → 19/10/2012
Number of participants: 5
Phd Student:
Tromholt, Thomas (Intern)
Main Supervisor:
Krebs, Frederik C (Intern)
Examiner:
Norby, Poul (Intern)
Nelson, Jenny (Ekstern)
Rivaton, Agnès (Ekstern)
**High Temperature Alkaline Electrolyser Cell**

Department of Energy Conversion and Storage  
Period: 15/05/2009 → 01/03/2013  
Number of participants: 7  
PhD Student: Allebrod, Frank (Intern)  
Supervisor: Ebbesen, Sune Dalgaard (Intern)  
Hjelm, Johan (Intern)  
Main Supervisor: Mogensen, Mogens Bjerg (Intern)  
Examiner: Holtappels, Peter (Intern)  
Skou, Eivind Morten (Ekstern)  
Sunde, Svein (Ekstern)

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Forskningsrådsfinansiering  
Project: PhD

**Electrochemical Reduction of NOx**

Department of Energy Conversion and Storage  
Period: 01/05/2009 → 27/06/2012  
Number of participants: 5  
PhD Student: Traulsen, Marie Lund (Intern)  
Main Supervisor: Kammer Hansen, Kent (Intern)  
Examiner: Holtappels, Peter (Intern)  
Rasmussen, Søren Birk (Intern)  
Skou, Eivind Morten (Ekstern)

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Offentlig finansiering  
Project: PhD

**A high performance ion transport membrane (HP-ITM)**

In the project HP-ITM, ion transport membranes (ITM) have been developed and oxygen fluxes of more than 5 ml min⁻¹ cm⁻² have been demonstrated. The project also documents potential limitations of the current demonstration pieces regarding mechanical strength of the ceramic supports and chemical expansion of the ceria based membrane materials.

Department of Energy Conversion and Storage  
Ceramic Engineering & Science  
Period: 01/04/2009 → 30/06/2010  
Number of participants: 1  
oxygen transport membranes, ceramic processing, tape casting  
Acronym: HP-ITM  
Number of related Ph.D. students: 1  
Project participant: Kaiser, Andreas (Intern)
Financing sources
Source: Public research council
Name of research programme: Proof of Concept for public research institutes
Amount: 966,439.04 Danish Kroner
Year of approval: 2007

Relations
Publications:
On the use of supported ceria membranes for oxyfuel process/syngas production
Oxygen permeation in thin, dense Ce0.9Gd0.1O 1.95- membranes II. experimental determination
Evaluation of thin film ceria membranes for syngas membrane reactors—Preparation, characterization and testing
Project

Development of 3D EBSD for characterisation of solid oxide electrolysis cells in relation to performance and degradation
Department of Energy Conversion and Storage
Period: 01/04/2009 → 30/09/2015
Number of participants: 6
Phd Student:
Saowadee, Nath (Intern)
Supervisor:
Agersted, Karsten (Ekstern)
Main Supervisor:
Bowen, Jacob R. (Intern)
Examiner:
Lauridsen, Erik Mejdal (Intern)
Gholinia, Ali (Ekstern)
Ringgaard, Erling (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Privatist
Project: PhD

Fremstilling og synteseanvendelse af elektrolytisk fremstillet hydrogen
Department of Energy Conversion and Storage
Period: 01/03/2009 → 23/05/2012
Number of participants: 7
Phd Student:
Hansen, Martin Kalmar (Intern)
Supervisor:
Christensen, Erik (Intern)
Jensen, Jens Oluf (Intern)
Main Supervisor:
Bjerrum, Niels J. (Intern)
Examiner:
Petrushina, Irina (Intern)
Bouzek, Karel (Ekstern)
Steenberg, Thomas (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.
Project: PhD

Cathodes for solid Oxide Fuel Cells Operating at 400 C
Department of Energy Conversion and Storage
Period: 15/02/2009 → 23/05/2012
Number of participants: 6
Phd Student:
Samson, Alfred Junio (Intern)
Supervisor:
Søgaard, Martin (Intern)
Main Supervisor:
Bonanos, Nikolaos (Intern)
Examiner:
Hagen, Anke (Intern)
Primdahl, Søren (Intern)
Serra-Alfaro, José Manuel (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut/centerfinansieret
Project: PhD

Anodes for SOFCs Operating at 400 degrees
Department of Energy Conversion and Storage
Period: 15/12/2008 → 18/04/2012
Number of participants: 6
Phd Student:
Abdul Jabbar, Mohammed Hussain (Intern)
Supervisor:
Høgh, Jens Valdemar Thorvald (Intern)
Main Supervisor:
Bonanos, Nikolaos (Intern)
Examiner:
Skaarup, Steen (Intern)
Boukamp, Bernard Abraham (Ekstern)
Skou, Eivind Morten (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut/centerfinansieret
Project: PhD

Computational methods for describing reaction rates at interfaces of energy materials
Department of Energy Conversion and Storage
Period: 01/12/2008 → 18/04/2012
Number of participants: 6
Phd Student:
Maronsson, Jon Bergmann (Intern)
Supervisor:
Jonsson, Hannes (Intern)
Main Supervisor:
Vegge, Tejs (Intern)
Examiner:
Rossmeisl, Jan (Intern)
Henkelman, Graeme (Ekstern)
Wahnström, Göran (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut/centerfinansieret
Project: PhD

3D Studies of Coarsening Kinetics of Individual Grains
Innovative solid oxide electrolyser stacks for efficient and reliable hydrogen production

The RelHy project targets the development of novel or improved, low cost materials (and the associated manufacturing process) for their integration in efficient and durable components for the next generation of electrolysers based on Solid Oxide Electrolysis Cells (SOEC). It is specifically tailored for 1) Optimisation of novel or improved cell, interconnect and sealing materials, 2) Achievement of innovative designs for SOE stacks to improve durability. As such, it is positioned as a bridge between currently good performing electrolysis cells and their efficient and reliable integration into advanced stacks to pave the way for the production of a new generation of electrolysers. To achieve these goals, the RelHy project is based on the coupled development of instrumented single repeat units and stacks and of associated simulation tools (from cell to stack scale). This mixed experimental and simulation approach will be used on several batches of materials -to give specifications for novel or improved materials and evaluate them, where special attention is paid to material compatibility (between electrodes, electrolyte, coating, interconnects and sealing). -to propose innovative designs able to overcome the present limiting parameters and to increase stack reliability, durability and performance. These material and design innovations will be validated at laboratory scale on a 25-cell stack prototype and its competitiveness will be assessed. Since the project is centered on R&D activities, the RelHy multidisciplinary European consortium is merging expertise from two university laboratories and three research centres already recognised for material development and cell production, instrumentation and testing, and modelling (DTU-Risoe, Imperial College, ECN, EIFER and CEA) and also from a fuel cell stack manufacturer that can produce electrolyser stacks (TOFC) and from an energy company (HELION) that can specify the operation conditions and assess the competitiveness of the innovative electrolyser prototype and its potential integration. The main issue addressed in the project is the simultaneous achievement of both, lifetime (degradation close to 1% for 1000 hr on single repeat units at 800°C) and efficiency (0.03 to 0.04 gH2/cm2/hr, i.e. approximately 1 A/cm2 with water utilisation >60% and a stack efficiency > 90%). These operation points and degradation values will yield an efficiency of up to 80% (LHV) at the system level with >99% availability. Cost issues will also be addressed by considering
cost effective materials and processes in order to meet the "non energy" 1€/kg H2 target.

Department of Energy Conversion and Storage

Applied Electrochemistry

Risø National Laboratory for Sustainable Energy

Fuel Cells and Solid State Chemistry Division

Electrochemical Evaluation

Electrochemistry
Period: 01/01/2008 → 31/12/2011
Number of participants: 3
High temperature electrolysis
Acronym: RelHy
Project participant:
Ebbesen, Sune Dalgaard (Intern)
Ehora, Ghislaine (Intern)

Project Manager, organisational:
Bowen, Jacob R. (Intern)

Financing sources
Source: Forsk. EU - Rammeprogram
Name of research programme: Forsk. EU - Rammeprogram
Amount: 4,733,454.00 Danish Kroner

Relations
Activities:
Microstructure characterisation of solid oxide electrolysis cells operated at high current density

Polymer Solar Cells for Solar Energy Conversion
DSF sagsnr.: 2104-07-0022, DTU projektnr.: 48010

Department of Energy Conversion and Storage

Functional organic materials
Period: 01/01/2008 → 31/12/2013
Number of participants: 1
Project Manager, academic:
Krebs, Frederik C (Intern)

Relations
Publications:
Solar Test Platform
Low band gap polymers for organic solar cells
Thermally reactive Thiazolo[5,4-d]thiazole based copolymers for high photochemical stability in polymer solar cells
Advanced Functional Polymers for Increasing the Stability of Organic Photovoltaics
Concentrated Light for Accelerated Photo Degradation of Polymer Materials
Non-destructive lateral mapping of the thickness of the photoactive layer in polymer-based solar cells
Aesthetically Pleasing Conjugated Polymer: Fullerene Blends for Blue-Green Solar Cells Via Roll-to-Roll Processing
Ambient fabrication of flexible and large-area organic light-emitting devices using slot-die coating
Application of optical coherence tomography (OCT) as a 3-dimensional imaging technique for roll-to-roll coated polymer solar cells
Comparative studies of photochemical cross-linking methods for stabilizing the bulk hetero-junction morphology in polymer solar cells
Enhancing functionality of ZnO hole blocking layer in organic photovoltaics
Exciton diffusion length in some thermocleavable polythiophenes by the surface photovoltage method
Influence of processing and intrinsic polymer parameters on photochemical stability of polythiophene thin films
Investigation of the degradation mechanisms of a variety of organic photovoltaic devices by combination of imaging techniques—the ISOS-3 inter-laboratory collaboration
Large-scale roll-to-roll photonic sintering of flexo printed silver nanoparticle electrodes
Low-temperature side-chain cleavage and decarboxylation of polythiophene esters by acid catalysis
New Low-Bandgap Materials with Good Stabilities and Efficiencies Comparable to P3HT in R2R-Coated Solar Cells
On the stability of a variety of organic photovoltaic devices by IPCE and in situ IPCE analyses – the ISOS-3 inter-laboratory collaboration
Photochemical stability of conjugated polymers, electron acceptors and blends for polymer solar cells resolved in terms of film thickness and absorbance
Roll-to-roll fabrication of polymer solar cells
Solar cells with one-day energy payback for the factories of the future
Stability of Polymer Solar Cells
The ISOS-3 inter-laboratory collaboration focused on the stability of a variety of organic photovoltaic devices
The use of polyurethane as encapsulating method for polymer solar cells—An inter laboratory study on outdoor stability in 8 countries
TOF-SIMS investigation of degradation pathways occurring in a variety of organic photovoltaic devices – the ISOS-3 inter-laboratory collaboration
A compact multi-chamber setup for degradation and lifetime studies of organic solar cells
A life cycle analysis of polymer solar cell modules prepared using roll-to-roll methods under ambient conditions
An inter-laboratory stability study of roll-to-roll coated flexible polymer solar modules
A self-calibrating led-based solar test platform
A solution process for inverted tandem solar cells
Consensus stability testing protocols for organic photovoltaic materials and devices
Degradation of semiconducting polymers by concentrated sunlight
Economic assessment of solar electricity production from organic-based photovoltaic modules in a domestic environment
Electrical and Photo-Induced Degradation of ZnO Layers in Organic Photovoltaics
Ellipsometry as a Nondestructive Depth Profiling Tool for Roll-to-Roll Manufactured Flexible Solar Cells
Fabrication of Polymer Solar Cells Using Aqueous Processing for All Layers Including the Metal Back Electrode
Fused thiophene/quinoxaline low band gap polymers for photovoltaic’s with increased photochemical stability
Life-cycle analysis of product integrated polymer solar cells
Origin of size effect on efficiency of organic photovoltaics
Oxygen- and water-induced degradation of an inverted polymer solar cell: the barrier effect
Photochemical stability and photovoltaic performance of low-band gap polymers based on dithiophene with different bridging atoms
Polymers for organic photovoltaics based on 1,5-bis(2-hexyldecyloxy)-naphthalene, thiophene, and benzothiadiazole
Business, market and intellectual property analysis of polymer solar cells
Water and oxygen induced degradation of small molecule organic solar cells
Roll-to-Roll Processing of Inverted Polymer Solar Cells using Hydrated Vanadium(V)Oxide as a PEDOT:PSS Replacement
Printed metal back electrodes for R2R fabricated polymer solar cells studied using the LBIC technique
Degradation Patterns in Water and Oxygen of an Inverted Polymer Solar Cell
Influence of the Annealing Temperature on the Photovoltaic Performance and Film Morphology Applying Novel Thermocleavable Materials
Low band gap polymers based on 1,4-dialkoxybenzene, thiophene, bithiophene donors and the benzothiadiazole acceptor
Low Band Gap Polymers for Roll-to-Roll Coated Polymer Solar Cells
Manufacture, integration and demonstration of polymer solar cells in a lamp for the Lighting Africa initiative
Photovoltaic Performance of Polymers Based on Dithienylthienopyrazines Bearing Thermocleavable Benzoate Esters
Product integration of compact roll-to-roll processed polymer solar cell modules: methods and manufacture using flexographic printing, slot-die coating and rotary screen printing
The effect of post-processing treatments on inflection points in current–voltage curves of roll-to-roll processed polymer photovoltaics
Thermo-cleavable polymers: Materials with enhanced photochemical stability
The teraton challenge. A review of fixation and transformation of carbon dioxide
Ultra Fast and Parsimonious Materials Screening for Polymer Solar Cells Using Differentially Pumped Slot-Die Coating
Upscaling of polymer solar cell fabrication using full roll-to-roll processing
Using Light-Induced Thermocleavage in a Roll-to-Roll Process for Polymer Solar Cells
All solution roll-to-roll processed polymer solar cells free from indium-tin-oxide and vacuum coating steps
A roll-to-roll process to flexible polymer solar cells: model studies, manufacture and operational stability studies
A round robin study of flexible large-area roll-to-roll processed polymer solar cell modules
Fabrication and processing of polymer solar cells: A review of printing and coating techniques
"Hairy" Poly(3-hexylthiophene) Particles Prepared via Surface-Initiated Kumada Catalyst-Transfer Polycondensation
Investigation of optical spacer layers from solution based precursors for polymer solar cells using X-ray reflectometry
Pad printing as a film forming technique for polymer solar cells
Polymer solar cell modules prepared using roll-to-roll methods: Knife-over-edge coating, slot-die coating and screen printing
Roll-to-roll fabrication of monolithic large-area polymer solar cells free from indium-tin-oxide
Study of hybrid solar cells made of multilayer nanocrystalline titania and poly(3-octylthiophene) or poly-(3-(2-methylhex-2-yl)-oxy-carbonyldithiophene)
Thermocleavable Materials for Polymer Solar Cells with High Open Circuit Voltage - A Comparative Study
Thermo-cleavable solvents for printing conjugated polymers: Application in polymer solar cells
Water-Induced Degradation of Polymer Solar Cells Studied by (H2O)-O-18 Labeling
Air stable polymer photovoltaics based on a process free from vacuum steps and fullerenes
All solution processed tandem polymer solar cells based on thermocleavable materials
An explanation for the high stability of poly(carboxy)thiophenes in photovoltaic devices - A solid-state NMR dipolar recoupling study
Applicability of X-ray reflectometry to studies of polymer solar cell degradation
A setup for studying stability and degradation of polymer solar cells
A simple nanostructured polymer/ZnO hybrid solar cell - preparation and operation in air
Biodegradable polymer solar cells
Bulk heterojunctions based on native polythiophene
Thermocleavable Low Band Gap Polymers and Solar Cells Therefrom with Remarkable Stability toward Oxygen
Structural and chemical investigation of CdSe crystals deposited in a nanoporous sol-gel: Effect of chemistry and defects on photovoltaic properties
Analysis of the failure mechanism for a stable organic photovoltaic during 10 000 h of testing
The OE-A OPV demonstrator anno domini 2011
Ultra high open circuit voltage (>1 V) of poly-3-hexylthiophene based organic solar cells with concentrated light
Polymer Solar Cells – Non Toxic Processing and Stable Polymer Photovoltaic Materials
Stability and Degradation of Organic and Polymer Solar Cells
Polymeric solar cells; materials, design, manufacture
Polymer photovoltaics: A practical approach
Organic solar cells
Characterization and Reporting of OPV Device Lifetime
Concentrated Light for Organic Photovoltaics
Degradation of Polymer-Based OPV
Polymers and sol cells
The Different PV Technologies and How They Degrade
Introduction
Manufacture
Market Analysis
Materials and Processing
Patent Overview of OPVs
Stability and Characterization of Devices
Technology Potential and Outlook
Introduction
Lifetime and stability studies
Outlook
Processing and production of large modules
The polymer solar cell
Photovoltaics efficiency improvements
Energy efficient Solid State Lighting
Solar energy
Combined Characterization Techniques to Understand the Stability of a Variety of Organic Photovoltaic Devices - the ISOS-3 inter-laboratory collaboration
Optical coherence tomography (OCT) as a 3-dimensional imaging technique for non-destructive testing of roll-to-roll coated polymer solar cells
Edge sealing for low cost stability enhancement of roll-to-roll processed flexible polymer solar cell modules
Interlayer adhesion in roll-to-roll processed flexible inverted polymer solar cells
Quality control of roll-to-roll processed polymer solar modules by complementary imaging methods
Simple roll coater with variable coating and temperature control for printed polymer solar cells
Stability and degradation of organic photovoltaics fabricated, aged, and characterized by the ISOS 3 inter-laboratory collaboration
Economical assessment of solar electricity from organic photovoltaic systems
Large area modules based on low band gap polymers
Polymer solar cells for solar energy conversion
Solar energy – new photovoltaic technologies
Improved adhesion of metal oxide layer
Improved electron transport layer
PROCES OF ELECTRICAL CONNECTION OF PHOTOVOLTAIC DEVICES
Photovoltaic device
Air Stable Photovoltaic Device
Method of Testing Solar Cells
Method of Thermocleaving a Polymer Layer
Editorial for the special issue on ISOS-3 (Third International Summit on OPV Stability)
Video editorial for the special issue on ISOS-3 (3rd international summit on OPV stability)
Editorial for the special issue on EMRS-A
Editorial: Reporting solar cell efficiencies in Solar Energy Materials and Solar Cells
Solceller lavet af plast
Project

Automatic Quantitative Image Analysis of 3D Micrographs
Department of Informatics and Mathematical Modeling
Department of Energy Conversion and Storage
Imaging and Structural Analysis
Period: 01/03/2007 → 22/09/2010
Number of participants: 7
Phd Student:
Jørgensen, Peter Stanley (Intern)
Supervisor:
Bowen, Jacob R. (Intern)
Hansen, Karin Vels (Intern)
Main Supervisor:
Larsen, Rasmus (Intern)
Examiner:
Bærentzen, Jakob Andreas (Intern)
Barnett, Scott (Intern)
Østergaard, Lasse Riis (Ekstern)
Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD
Development of software for the analysis of positron lifetime spectra
Department of Energy Conversion and Storage

Atomic scale modelling and materials
Period: 01/01/2007 → …
Number of participants: 3
PALSfit
Acronym: PALSfit
Project participant:
Eldrup, Morten Mostgaard (Intern)
Kirkegaard, Peter (Intern)
Olsen, Jens V. (Intern)

PALSfit

Acronym: PALSfit

Project participant:
Eldrup, Morten Mostgaard (Intern)
Kirkegaard, Peter (Intern)
Olsen, Jens V. (Intern)

Project

Resistance of Ni-Cermet anode supports against reduction-oxidation cycling: a step towards better durability of solid oxide fuel cells
Solid oxide fuel cells (SOFC) are a promising energy technology suitable for clean and efficient direct conversion of hydrogen carrying fuels into electricity and heat. The main potential market areas of SOFC systems are within distributed energy generation (combined heat and power) from small Residential applications up to MW class, and Auxiliary Power Units (APU) for both land and marine transport. The SOFC technology is currently under intensive research and development with an expected market entry of products within 1-3 years. Research and development are directed towards reducing cell and system cost, and improving the performance and durability of the cells under operation. The current project tackles the durability issue with the focus on a practical problem related to the operation of most current SOFC cells or systems, the so-called RedOx stability (= stability after a cycle of re-oxidation and reduction of an operating cell). The state-of-the-art SOFC anode is made of a composite of nickel and yttria stabilised zirconia. The anode supported cell design is operating at temperatures of 700-800 degrees Celsius with reducing atmosphere on the anode side. Due to cost issues, many small scale SOFC systems are not expected to have an inert sweep gas supply. In the case of fuel interruption, an oxidation of the nickel at these temperatures either severely degrades or completely destroys most current cells. The destruction is induced by the macroscopic expansion of the anode support, which results in destruction of the support itself and by cracking of the supported electrolyte layer. The large volumetric expansion is mainly caused by the phase change from Ni to NiO, which is the so-called redox instability. The aim of the project has been to better understand the mechanisms and processes related to redox instability and through modifications to the half cell to improve the RedOx stability of Ni-based SOFC. We have demonstrated a redox stable Ni-YSZ composite and are in the process of implementing a modified structure into technologically relevant half cells. We have followed a pre-defined track of development work aiming to find microstructures and/or compositions that enable more stable structures under a variety of operation conditions. In simple terms the redox instability is a thermo mechanical problem: excessive stresses in the layered ceramic cell structure may cause cracking and loss of tightness of the cell, with the electrolyte being the critical component. In the anode supported SOFC, the origin of the stress exerted on the electrolyte is the dimensional expansion of the anode support on re-oxidation. Therefore, the main goal of the development work was to design and manufacture anode substrates with improved dimensional stability during redox cycling. The target level, based on literature, was set to a linear expansion of 0.1 % on re-oxidation. The current anode substrate could not reach this target even at the mildest conditions. As a result of the project, we have gained an improved understanding on the processes of importance during redox cycling. We designed and manufactured several modified anode support substrates and the best of these reach the stability target of 0.1 % maximum expansion after 3 redox cycles at 850 oC under certain conditions. These results were based on modifications in the composite microstructure and composition by ceramic processing, by changing the sizes and distributions of particles and pores in the composite. Dopants were added to the nickel phase to improve the creep resistance and suppress nickel grain growth during operation or redox cycling. Within the project it was difficult to fully prove the effectiveness of these dopants compared to simultaneously introduced changes in microstructure. The implementation of the best modified anode support structures in technological half cells was started within this project. While knowledge about an improved anode support structure were obtained, further work in ceramic processing, mainly related to understanding sintering and co-sintering, is still needed to implement these structures in technologically relevant cells.
Number of related Ph.D. students: 1
Project participant:
Kaiser, Andreas (Intern)

Financing sources
Source: EU research programme (public)
Name of research programme: FP6-Mobility
Amount: 189,549.00 Euro
Year of approval: 2006

Relations
Publications:
- Strength of Anode-Supported Solid Oxide Fuel Cells
- Continuum mechanics simulations of NiO/Ni-YSZ composites during reduction and re-oxidation
- Curvature and Strength of Ni-YSZ Solid Oxide Half-Cells After Redox Treatments
- Redox stability of SOFC: Thermal analysis of Ni-YSZ composites
- Dimensional behaviour of Ni-YSZ anode supports for SOFC under redox cycling conditions
- Testing and improving the redox stability of Ni-based SOFC
- Mechanical properties of NiO/Ni-YSZ composites depending on temperature, porosity and redox cycling
- Dimensional behavior of Ni-YSZ composites during redox cycling
- Electrical conductivity of Ni–YSZ composites: Variants and redox cycling

Documents:
- Thesis-Mikko-Pihlatie-P740
- CORDIS_result_49143_en

Activities:

Cerâmica (Journal)
Period: 2018
Vincenzo Esposito (Editor)
Department of Energy Conversion and Storage

Related journal
Cerâmica
0366-6913
Scopus rating (2017): CiteScore 0.44 SJR 0.186 SNIP 0.365
Indexed in DOAJ

Activity: Research › Journal editor

Period: 19 Aug 2018 → 24 Aug 2018
Ngo Van Nong (Organizer)
Department of Energy Conversion and Storage
Ceramic Engineering & Science

Related event
19/08/2018 → …
Daejeon, Korea, Democratic People’s Republic of
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Journal of Electronic Materials (Journal)
Period: Jul 2018 → Dec 2018
Improving Co-free oxygen electrodes for solid oxide cells through surface modification
Period: 9 Jul 2018 → 12 Jul 2018
Dordije Tripkovic (Guest lecturer)
Jiayue Wang (Other)
Roland Bliem (Other)
Bilge Yildiz (Guest lecturer)
Mogens Bjerg Mogensen (Guest lecturer)
Peter Vang Hendriksen (Guest lecturer)

Mixed Conductors
Electrochemical Materials and Interfaces
Degree of recognition: International

Electroceramics XVI abstract - Dordije Tripkovic

CuMn foam as air side contact layer – interface adhesion and area specific resistance after aging
Period: 3 Jul 2018 → 6 Jul 2018
Belma Talic (Other)
Li Han (Other)
Philipp Zielke (Other)
Anders Christian Wulff (Other)
Peter Vang Hendriksen (Other)
Henrik Lund Frandsen (Other)

13th European Fuel Cell Forum
03/07/2018 → 06/07/2018
Luzern, Switzerland
Activity: Talks and presentations › Conference presentations
Galvanostatic and potentiostatic operation of real landfill gas fueled SOFCs
Period: 3 Jul 2018 → 6 Jul 2018
Hendrik Langnickel (Guest lecturer)
Christopher R. Graves (Guest lecturer)
Anke Hagen (Guest lecturer)
Department of Energy Conversion and Storage
Applied Electrochemistry
Degree of recognition: International

Related event
13th EUROPEAN SOFC & SOE FORUM
03/07/2018 → 06/07/2018
Lucerne, Switzerland
Activity: Talks and presentations › Conference presentations

Thermal building mass for storage and its role in smart energy systems
Period: 1 Jul 2018
Dominik Franjo Dominkovic (Speaker)
Department of Energy Conversion and Storage
Energy Systems Analysis
Degree of recognition: International

Related event
3rd South east European SDEWES Conference
30/06/2018 → 04/07/2018
Novi Sad, Serbia
Activity: Talks and presentations › Conference presentations

SCANDEM 2018 - The 69th Annual Conference of the Nordic Microscopy Society
Period: 25 Jun 2018 → 28 Jun 2018
Jacob R. Bowen (Organizer)
Department of Energy Conversion and Storage
Imaging and Structural Analysis
Description
Materials Science and Energy Materials - Session Organiser, Session Chair
Degree of recognition: International
Links:
https://issuu.com/dtudanchipcen/docs/scandem-program-web_250618 (Programme)

Related event
SCANDEM 2018 - The 69th Annual Conference of the Nordic Microscopy Society
25/06/2018 → 28/06/2018
Kgs. Lyngby, Denmark
Activity: Attending an event › Participating in or organising a conference

Sample Design and Preparation Techniques for Dynamic Microstructural Studies of High Temperature Electrochemical Cells
Period: 11 Jun 2018
Jacob R. Bowen (Speaker)
Department of Energy Conversion and Storage
Imaging and Structural Analysis

**Description**
Understanding the dynamics of 3D microstructural change in high temperature electrochemical cells, primarily solid oxide fuel cells or electrolyzers, is a pressing driving force for performing time resolved ex-situ, in-situ and in-operando nano-tomography and diffraction based experiments at synchrotron X-ray sources. These experiments must meet simultaneous challenging demands: precision beamline compatible samples that are stable at high temperature, supply of electric potential, and control of atmosphere. Correct sample design is an absolute necessity for experimental success. Here, the merits of possible sample configurations and environments are explored and evaluated against fabrication challenges and experimental feasibility. Experience with designing and performing experiments of selected configurations will be presented. Results of 3D nano-tomography of Ni-yttria stabilized zirconia (YSZ) fuel electrode microstructure evolution during Ni oxidation, reduction and annealing, and spatially resolved in-operando diffraction studies of YSZ electrolytes under at high polarization will be summarised.

Degree of recognition: International

**Related organisation**

Sample Design and Preparation Techniques for Dynamic Microstructural Studies of High Temperature Electrochemical Cells
Bowen, J. R. (Speaker)
11 Jun 2018
Activity: Talks and presentations › Conference presentations

Time-resolved X-ray Absorption Spectroscopy of Copper Zinc Tin Sulfide Nanoparticles
Period: 6 Jun 2018
Christian Rein (Guest lecturer)
Department of Energy Conversion and Storage
Imaging and Structural Analysis
Degree of recognition: National
Documents:
DFS 2018 - Time-resolved X-ray Absorption Spectroscopy of Copper Zinc Tin Sulfide

Related event
Annual Meeting of Danish Physical Society 2018
06/06/2018 → 07/07/2018
Denmark
Activity: Talks and presentations › Conference presentations

High performance thermoelectric materials and modules for energy harvesting
Period: 26 Apr 2018
Ngo Van Nong (Guest lecturer)
Department of Energy Conversion and Storage
Ceramic Engineering & Science

Related event
Thermoelectrics - from fundamentals to applications
26/04/2018 → …
Oslo, Norway
Activity: Talks and presentations › Conference presentations

PhD thesis "Stability and properties of materials and interfaces for oxide thermoelectrics"
Period: 25 Apr 2018
Ngo Van Nong (External examiner)
Department of Energy Conversion and Storage
Ceramic Engineering & Science
Atomistic studies of anode and cathode materials for zinc-air batteries
Period: 11 Apr 2018
Steen Lysgaard (Guest lecturer)
Department of Energy Conversion and Storage
Atomic scale modelling and materials
Degree of recognition: International

Related event
Second International Zn-Air Battery Workshop
11/04/2018 → 12/04/2018
Trondheim, Norway
Activity: Talks and presentations › Conference presentations

Magnetic Refrigeration for Near Room-Temperature applications
Period: 9 Apr 2018
Kurt Engelbrecht (External examiner)
Department of Energy Conversion and Storage
Electrofunctional materials

Description
PhD pre-defense at KTH
Degree of recognition: International
Activity: Examinations and supervision › External examination

2018 MIT energy conference
Period: 2 Mar 2018 → 3 Mar 2018
Dominik Franjo Dominkovic (Participant)
Department of Energy Conversion and Storage
Energy Systems Analysis

Related event
2018 MIT energy conference
02/03/2018 → 03/03/2018
Boston, United States
Activity: Attending an event › Participating in or organising a conference

Sustainable synthetic fuels from biomass gasification and electrolysis
Period: 2 Mar 2018 → 3 Mar 2018
Dordije Tripkovic (Guest lecturer)
Department of Energy Conversion and Storage
Mixed Conductors

Description
Poster presentation
Degree of recognition: International
Documents:
Sustainable synthetic fuels from biomass gasification and electrolysis - Poster

Related event
2018 MIT energy conference
02/03/2018 → 03/03/2018
**Which storage types are needed in future smart energy cities?**

**Period:** 29 Jan 2018  
**Dominik Franjo Dominkovic (Speaker)**  
**Department of Energy Conversion and Storage**  
**Energy Systems Analysis**  
**Degree of recognition:** International

**Related event**

**1st Latin American SDEWES Conference**  
28/01/2018 → 31/01/2018  
Rio de Janeiro, Brazil  
Activity: Talks and presentations › Conference presentations

**Correlating Oxygen Electrode Degradation to Cr Vaporization from Metallic Interconnects in Solid Oxide Cell Stacks**

**Period:** 25 Jan 2018  
**Belma Talic (Speaker)**  
**Peter Vang Hendriksen (Other)**  
**Department of Energy Conversion and Storage**  
**Mixed Conductors**

**Description**  
Oral Contribution  
**Degree of recognition:** International  
**Documents:**  
ICACC 2018 abstract TALIC

**Related event**

**42nd International Conference and Exposition on Advanced Ceramics and Composites**  
21/01/2018 → 26/01/2018  
Daytona Beach, United States  
Activity: Talks and presentations › Conference presentations

**Microstructural and electrical characterization of Cu and Fe-doped Mn-Co spinel protective coatings for solid oxide cell interconnects**

**Period:** 24 Jan 2018  
**Federico Smeacetto (Speaker)**  
**Antonio G. Sabato (Other)**  
**Hassan Javed (Other)**  
**Belma Talic (Other)**  
**Sebastian Molin (Other)**  
**Department of Energy Conversion and Storage**  
**Mixed Conductors**

**Description**  
Contributed (Oral) presentation  
**Degree of recognition:** International  
**Documents:**  
ICACC 2018 abstract SMEACETTO

**Related event**

**42nd International Conference and Exposition on Advanced Ceramics and Composites**  
21/01/2018 → 26/01/2018
Daytona Beach, United States
Activity: Talks and presentations › Conference presentations

**National Renewable Energy Laboratory**
Period: 4 Jan 2018 → 22 Apr 2018
Dominik Franjo Dominkovic (Visiting researcher)
Department of Energy Conversion and Storage
Energy Systems Analysis

**Description**
Guest research stay that lasted for 3.5 months. The guest research stay took place at NREL, Golden, Colorado, the USA. I was working on integrated energy modelling of Aruba, an island-nation located in the Caribbean.
Degree of recognition: International
Activity: Visiting another research institution

**Journal of Power Sources (Journal)**
Period: 2017
Anke Hagen (Reviewer)
Department of Energy Conversion and Storage
Applied Electrochemistry

**Related journal**
Journal of Power Sources
0378-7753
Central database
Activity: Research › Peer review of manuscripts

**Wissenschaftsfonds FWF (Fonds zur Förderung der wissenschaftlichen Forschung) Österreichs (External organisation)**
Period: 2017
Anke Hagen (Chairman)
Department of Energy Conversion and Storage
Applied Electrochemistry

**Description**
Evaluation of proposals

**Related external organisation**
Wissenschaftsfonds FWF (Fonds zur Förderung der wissenschaftlichen Forschung) Österreichs
Austria
Activity: Membership › Membership in review committee

**Operation of real landfill gas fueled solid oxide fuel cell (SOFC) using internal dry reforming**
Period: 12 Dec 2017 → 15 Dec 2017
Hendrik Langnickel (Guest lecturer)
Anke Hagen (Guest lecturer)
Department of Energy Conversion and Storage
Applied Electrochemistry

**Description**
It is generally agreed that due to the increasing amount of renewable energy in the electricity production different energy conversion and storage technologies are needed to ensure a 100% availability of electricity.
Considering biomass as renewable source, fuel derived from landfill appears as attractive option. Landfill gas consists of carbon dioxide, methane and impurities as for example sulfur containing compounds. Combustion engines are often used
to convert landfill gas into electricity and heat with the disadvantages of low efficiencies. Furthermore, most landfill gases are unattractive for combustion engines due to their low heating values.

One option to utilize landfill gases with a low heating value and to increase the electrical efficiency is the solid oxide fuel cell (SOFC). With SOFCs it is possible to convert hydrogen or carbon containing fuels, as for example landfill gas, directly into electricity and the side product heat in a highly efficient way.

To convert the landfill gas directly into electricity and heat in an SOFC, a reforming agent is needed to prevent carbon formation. Beside steam, it is possible to use carbon dioxide as a reforming agent (dry reforming). The advantage is that landfill gas already contains a certain amount of the needed carbon dioxide.

In the present work a planar 16 cm² SOFC cell was operated with a real landfill gas from one of the largest Danish waste dump sites and additional carbon dioxide reforming agent at 750 °C, both with gas cleaning through an active carbon filter and without. The tests showed an electric efficiency up to 60%. It was found that the active carbon filter was necessary to prevent poisoning and thereby to decrease the degradation rate.

Degree of recognition: International

Links:

Related event
7th European Fuel Cell Piero Lunghi Conference
12/12/2017 → 16/12/2017
Naples, Italy
Activity: Talks and presentations › Conference presentations

Reversible Operation using Carbonaceous Gasses of a 30-cell Solid Oxide Cell Stack
Period: 12 Dec 2017 → 15 Dec 2017
Søren Højgaard Jensen (Guest lecturer)
Hendrik Langnickel (Guest lecturer)
Nils Hintzen (Other)
Ming Chen (Guest lecturer)
Xiufu Sun (Guest lecturer)
Anne Hauch (Guest lecturer)
Giacomo Butera (Guest lecturer)
Lasse Røngaard Clausen (Guest lecturer)
Department of Energy Conversion and Storage
Applied Electrochemistry
Mixed Conductors
Department of Mechanical Engineering
Thermal Energy

Description
Recent theoretical studies show that reversible electrochemical conversion of H2O and CO2 to CH4 inside novel pressurized solid oxide cells (SOCs) combined with subsurface storage of the produced gasses can facilitate seasonal electricity storage with a round-trip efficiency 70-80% and a storage cost below 3 ¢/kWh. Here we show test results from a 30-cell SOC stack operated with carbonaceous gasses at 18.7 bar at 700 °C in both electrolysis and fuel cell mode. The GC data from the electrolysis test results show 18% methane in the dry outlet gas, i.e. substantial methane formation inside the SOC stack. Further we observed degradation rates comparable to that of ambient pressure operation with H2/H2O gas mixtures.

Links:
Related event

7th European Fuel Cell Piero Lunghi Conference
12/12/2017 → 16/12/2017
Naples, Italy
Activity: Talks and presentations › Conference presentations

Towards solid oxide electrolysis plants in 2020
Period: 28 Nov 2017
Ming Chen (Other)
Department of Energy Conversion and Storage
Mixed Conductors
Description
Poster presentation
Degree of recognition: National

Related event

Den danske brint-og brændselscelledag 2017
28/11/2017 → 28/11/2017
Odense, Denmark
Activity: Talks and presentations › Conference presentations

In-operando observation of microstructural evolution in a solid oxide cell electrolyte operating at high polarisation
Period: 17 Nov 2017
Jose Xavier Sierra Trujillo (Speaker)
Department of Energy Conversion and Storage
Imaging and Structural Analysis
Description
Oral presentation about some of the results of the PhD project.
Degree of recognition: Local
Documents:
DTU PhD Symposium JXST 2017

Related event

DTU Energy's annual PhD symposium 2017
17/11/2017 → 17/11/2017
Kgs. Lyngby, Denmark
Activity: Talks and presentations › Conference presentations

Wilson K. S. Chiu
Start date: 14 Nov 2017
Jacob R. Bowen (Host)
Department of Energy Conversion and Storage
Imaging and Structural Analysis
Description
Synchrotron-based Hard X-Ray Microscopy: A Tool for 3-D Spectroscopic Imaging at the Nanoscale
Degree of recognition: International
Activity: Hosting a guest lecturer

Gerardina Carbone
Start date: 13 Nov 2017
Jacob R. Bowen (Host)
Department of Energy Conversion and Storage
Imaging and Structural Analysis

**Description**
Brilliant opportunities with X-ray Nanobeams
Degree of recognition: **International**
Documents:
DTU_DCarbone_Nov17
Activity: Hosting a guest lecturer

**Development of Oxygen Electrodes for High Temperature and Pressure Alkaline Electrolysis Cells (HTP-AEC)**
Period: 3 Nov 2017
Jens Quitzau Adolphsen (Guest lecturer)
Department of Energy Conversion and Storage
Ceramic Engineering & Science

**Description**
Oral Presentation given on the conference
Documents:
DEF2017_jenqui

**Related event**
**Electrochemical Science and Technology Conference 2017**
02/11/2017 → 03/11/2017
Kgs. Lyngby, Denmark
Activity: Talks and presentations › Conference presentations

**Perspectives in alkaline water electrolysis using membranes**
Period: 3 Nov 2017
Mikkel Rykær Kraglund (Speaker)
Department of Energy Conversion and Storage
Proton conductors
Degree of recognition: **National**
Documents:
DEF_PorouZ_JOEL_LTalk-projects

**Related event**
**DEF Annual Meeting 2017**
02/11/2017 → 03/11/2017
Kgs. Lyngby, Denmark
Activity: Talks and presentations › Conference presentations

**Development of Oxygen Electrodes for High Temperature and Pressure Alkaline Electrolysis Cells (HTP-AEC)**
Period: 2 Nov 2017 → 3 Nov 2017
Jens Quitzau Adolphsen (Speaker)
Bhaskar Reddy Sudireddy (Guest lecturer)
Vanesa Gil (Guest lecturer)
Christodoulos Chatzichristodoulou (Guest lecturer)
Department of Energy Conversion and Storage
Ceramic Engineering & Science
Electrochemical Materials and Interfaces
Degree of recognition: **International**
Documents:
DEF2017_jenqui
**Related event**

**Electrochemical Science and Technology Conference 2017**  
02/11/2017 → 03/11/2017  
Kgs. Lyngby, Denmark  
Activity: Talks and presentations › Conference presentations

---

**Keramiske membraner til lutblæst forgasning**  
**Period:** 1 Nov 2017  
Astri Bjørnetun Haugen (Invited speaker)  
Department of Energy Conversion and Storage  
Ceramic Engineering & Science

**Description**  
Arranger: IDA Mechanical  
Degree of recognition: National  
Links:  

---

**Related event**

**UDVIKLING AF FREMTIDIGE METODER TIL PRODUKTION AF BIOBRÆNDSTOFFER OG GRØN ENERGI**  
01/11/2017 → …  
Aarhus, Denmark  
Activity: Talks and presentations › Conference presentations

---

**Advanced Concepts in Photovoltaics**  
**Period:** 10 Oct 2017 → 13 Oct 2017  
Peter Behrensdorff Poulsen (Organizer)  
Gisele Alves dos Reis Benatto (Organizer)  
Jørgen Schou (Organizer)  
Department of Photonics Engineering  
Optical Microsensors and Micromaterials  
Organic Energy Materials

**Description**  
Top Danish Researchers within photovoltaics was lecturing in this 4 day summer school along with Professor Peter Würfel, who is one of the international leading researchers within photovoltaics and author of the book Physics of Solar Cells: From Basic Principles to Advanced Concepts. The summer school was tailored towards PhD students within photovoltaics, but other interested in the program could join.  
Degree of recognition: International

---

**Related event**

**Advanced Concepts in Photovoltaics: A Summer School in Photovoltaics**  
10/10/2017 → 13/10/2017  
Roskilde, Denmark  
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

---

**Progress in Photovoltaic Research in Denmark 2017**  
**Period:** 9 Oct 2017  
Peter Behrensdorff Poulsen (Organizer)  
Gisele Alves dos Reis Benatto (Organizer)  
Department of Photonics Engineering  
Optical Microsensors and Micromaterials
Organic Energy Materials

Description
For the conference we had assembled all the top researchers in Denmark within Photovoltaics to tell about their latest results. Furthermore, some of the highly innovative companies within photovoltaics in Denmark did elaborate on their newest achievements.
Degree of recognition: International

Related event

**Progress in Photovoltaic Research in Denmark 2017: Conference i Photovoltaics**
09/10/2017 → ...
Roskilde, Denmark
Activity: Attending an event › Participating in or organising a conference

**12th International SDEWES Conference**
Period: 6 Oct 2017
Dominik Franjo Dominkovic (Speaker)
Department of Energy Conversion and Storage
Description
Held a presentation on: Integration of district cooling in smart energy systems: the case of Singapore
Degree of recognition: International

Related event

**12th sdewes Conference**
04/10/2017 → 08/10/2017
Dubrovnik, Croatia
Activity: Talks and presentations › Conference presentations

**Advanced fabrication of porous ceramic multilayers for membrane applications**
Period: 2 Oct 2017
Andreas Kaiser (Keynote speaker)
Wenjing (Angela) Zhang (Invited speaker)
Manuel Pinelo (Invited speaker)
Michela Della Negra (Other)
Department of Energy Conversion and Storage
Ceramic Engineering & Science
Proton conductors
Department of Chemical and Biochemical Engineering
Center for BioProcess Engineering
Degree of recognition: International
Documents:
Icm 2017 - abstract - Andreas Kaiser

Related organisation

**Advanced fabrication of porous ceramic multilayers for membrane applications**
Kaiser, A. (Keynote speaker), Zhang, W. (. (Invited speaker), Pinelo, M. (Invited speaker), Della Negra, M. (Other)
2 Oct 2017
Activity: Talks and presentations › Conference presentations

**Capillary-Based Micro-Battery Cells for Operando X-Ray Diffraction Studies of Electrode Materials in Working Li-Ion Batteries**
Period: 1 Oct 2017 → 5 Oct 2017
Rune E. Johnsen (Speaker)
In situ TEM study of the coarsening of carbon black supported Pt nanoparticles in hydrogen

Period: 1 Oct 2017 → 5 Oct 2017

Søren Bredmose Simonsen (Speaker)

Department of Energy Conversion and Storage
Imaging and Structural Analysis

Description
The control of sizes and shapes of nanostructures is of tremendous importance for the catalytic activity in electrochemistry and in catalysis more generally. However, due to relatively large surface free energies, nanostructures often sinter to form coarser and more stable structures that may not have the intended physicochemical properties.

Pt is known to be a very active catalyst in several chemical reactions and for example as carbon supported nanoparticles in fuel cells.

The presentation focusses on coarsening mechanisms of Pt nanoparticles supported on carbon black during exposure to hydrogen. By means of in situ transmission electron microscopy (TEM), Pt nanoparticle coarsening was monitored in 6 mbar 20 % H2/Ar while ramping up the temperature to ca. 900 °C. Time-resolved TEM images directly reveal that separated ca. 3 nm sized Pt nanoparticles in the pure hydrogen environment are stable during constant temperature ramping by 10°C/min up to ca. 800 °C. The coarsening above this temperature is fully dominated by the particle migration and coalescence mechanism. This is contrary to supported Pt nanoparticles in oxygen, where the coarsening is fully dominated by Ostwald ripening. For agglomerated Pt nanoparticles, coalescence events were observed already at ca. 200 °C. The temperature-dependency of particle sizes and the observed migration distances are consistent with simple early models for the migration and coalescence.

Degree of recognition: International

Related event
232nd ECS meeting
01/10/2017 → 05/10/2017
National Harbor, Washington, DC, United States
Activity: Talks and presentations › Conference presentations

The Atomic Simulation Environment and genetic algorithms
Period: 28 Sep 2017

Steen Lysgaard (Guest lecturer)

Department of Energy Conversion and Storage
Atomic scale modelling and materials
Degree of recognition: International

Related event
232nd ECS meeting
01/10/2017 → 05/10/2017
National Harbor, Washington, DC, United States
Activity: Talks and presentations › Conference presentations

NOMAD Summer: A hands-on course on tools for novel-materials discovery
Period: 25 Sep 2017 → 29 Sep 2017

Simon Loftager (Participant)
Department of Energy Conversion and Storage

Atomic scale modelling and materials
Degree of recognition: International

Related event

NOMAD Summer: A hands-on course on tools for novel-materials discovery
25/09/2017 → 29/09/2017
Berlin, Germany
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Fuel Cells (Journal)
Period: Aug 2017
Anke Hagen (Reviewer)
Department of Energy Conversion and Storage
Applied Electrochemistry
Links:

Related journal

Fuel Cells
1615-6846
BFI (2018): BFI-level 1, Scopus rating (2017): CiteScore 1.88 SJR 0.559 SNIP 0.748, ISI indexed (2013): ISI indexed yes, Web of Science (2018): Indexed yes
Central database
Activity: Communication › Journal editor

SOFC/battery powered electrical vehicle
Period: Aug 2017 → Dec 2017
Anke Hagen (External examiner)
Department of Energy Conversion and Storage
Applied Electrochemistry

Description
European Master in Renewable Energy
Activity: Examinations and supervision › Supervisor activities

Anode Catalyst Layer Contributing to the Overall Impedance of Polymer Electrolyte Membrane Electrolysis Cells during Water Electrolysis - A Hypothesis
Period: 30 Aug 2017
Katrine Elsøe (Guest lecturer)
Department of Energy Conversion and Storage

Related event

68th Annual Meeting of the International Society of Electrochemistry : Electrochemistry without Borders
27/08/2017 → 01/09/2017
Providence, United States
Activity: Talks and presentations › Conference presentations

The 15th International Conference on Advanced Materials IUMRS-ICAM
Period: 27 Aug 2017 → 1 Sep 2017
Ngo Van Nong (Organizer)
Department of Energy Conversion and Storage
Electrofunctional materials

Related event

The 15th International Conference on Advanced Materials IUMRS-ICAM
27/08/2017 → …
Kyoto, Japan
Activity: Attending an event › Participating in or organising a conference

NOVEL MATERIALS FOR MORE ROBUST SOLID OXIDE FUEL CELLS IN SMALL SCALE APPLICATIONS
Period: 21 Aug 2017
Peter Holtappels (Invited speaker)
Department of Energy Conversion and Storage
Degree of recognition: International
Documents:
IMRC24_2017_Holtappels_Novel materials for SOFC anodes_rev

Related event

24th International Materials Research Congress 2017
20/08/2017 → 25/08/2017
Cancun, Mexico
Activity: Talks and presentations › Conference presentations

Blockchain Summer School 2017
Period: 14 Aug 2017 → 18 Aug 2017
Dominik Franjo Dominkovic (Participant)
Department of Energy Conversion and Storage
Description
Successfully participated in the summer school
Degree of recognition: International

Related event

Blockchain Summer School 2017
14/08/2017 → 18/08/2017
Copenhagen, Denmark
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Progress of SOFC/SOEC Development at DTU Energy: From Materials to Systems
Period: Jul 2017
Anke Hagen (Guest lecturer)
Peter Vang Hendriksen (Other)
Department of Energy Conversion and Storage
Applied Electrochemistry
Mixed Conductors

Related event

15th International Symposium on Solid Oxide Fuel Cells (SOFC-XV)
23/07/2017 → 28/07/2017
Hollywood, United States
Activity: Talks and presentations › Conference presentations

Thermoneutral Operation of Solid Oxide Electrolysis Cells in Potentiostatic Mode
Period: 23 Jul 2017 → 28 Jul 2017
Ming Chen (Other)
Department of Energy Conversion and Storage

Mixed Conductors

Description
Poster presentation.
Degree of recognition: International

Related event
15th International Symposium on Solid Oxide Fuel Cells (SOFC-XV)
23/07/2017 → 28/07/2017
Hollywood, United States
Activity: Talks and presentations › Conference presentations

Materials Optimization Using Advanced Computational Methods
Period: 17 Jul 2017
Heine Anton Hansen (Invited speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials
Degree of recognition: International

Related event
16/07/2017 → 21/12/2017
Easton, United States
Activity: Talks and presentations › Conference presentations

Borohydride for Batteries
Period: 16 Jul 2017 → 21 Jul 2017
Didier Blanchard (Panel member)
Department of Energy Conversion and Storage
Degree of recognition: International

Related event
16/07/2017 → 21/07/2017
Easton, United States
Activity: Talks and presentations › Conference presentations

Climate-KIC PhD Summer School Urban Transition Amsterdam-Bologna 2017
Period: 16 Jul 2017 → 30 Jul 2017
Dominik Franjo Dominkovic (Participant)
Department of Energy Conversion and Storage

Description
Successfully participated in the summer school.
Degree of recognition: International

Related event
Climate-KIC PhD Summer School Urban Transition Amsterdam-Bologna 2017
16/07/2017 → 30/07/2017
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Development of Porous LaNi0.6Fe0.4O3 Electrodes with Tailored Microstructure for High Temperature and Pressure Alkaline Electrolysis Cells
Period: 12 Jul 2017
Jens Quitzau Adolphsen (Guest lecturer)
Department of Energy Conversion and Storage
Ceramic Engineering & Science

Description
Oral Presentation during the conference.
Degree of recognition: International
Documents:
ECerS2017 presentation 20170713-JensQAdolphsen

Related event
ECerS 2017 - 15th Conference & Exhibition of the European Ceramic Society
09/07/2017 → 13/07/2017
Budapest, Hungary
Activity: Talks and presentations › Conference presentations

Advanced manufacturing of porous ceramic structures for use in energy applications
Period: 10 Jul 2017
Andreas Kaiser (Invited speaker)
Department of Energy Conversion and Storage
Ceramic Engineering & Science
Degree of recognition: International
Documents:
ecers2017-abstract-Andreas Kaiser
Links:

Related event
ECerS 2017 - 15th Conference & Exhibition of the European Ceramic Society
09/07/2017 → 13/07/2017
Budapest, Hungary
Activity: Talks and presentations › Conference presentations

Development of Porous LaNi0.6Fe0.4O3 Electrodes with tailored microstructure for High Temperature and Pressure Alkaline Electrolysis Cells
Period: 9 Jul 2017 → 13 Jul 2017
Jens Quitzau Adolphsen (Speaker)
Bhaskar Reddy Sudireddy (Other)
Vanesa Gil (Other)
Christodoulos Chatziachristodoulou (Other)
Lennart Bergström (Other)
Department of Energy Conversion and Storage
Ceramic Engineering & Science
Electrochemical Materials and Interfaces
Degree of recognition: International
Documents:
ECerS2017 presentation 20170713-JensQAdolphsen

Related event
ECerS 2017 - 15th Conference & Exhibition of the European Ceramic Society
09/07/2017 → 13/07/2017
Budapest, Hungary
Activity: Talks and presentations › Conference presentations
30th International Conference on Efficiency, Cost, Optimization, Simulation and Environmental Impact of Energy Systems
Period: 5 Jul 2017
Dominik Franjo Dominkovic (Speaker)
Department of Energy Conversion and Storage

Description
Gave a presentation on: "A multi-objective energy planning including system exergy efficiency and socio-economic costs"
Degree of recognition: International

Related event

02/07/2017 → 06/07/2017
San Diego, United States
Activity: Talks and presentations › Conference presentations

3D Microstructural Evolution of a Solid Oxide Cell during a Redox Cycle by High Resolution Ptychographic Tomography
Period: 28 Jun 2017
Salvatore De Angelis (Guest lecturer)
Department of Energy Conversion and Storage
Imaging and Structural Analysis

Description
3rd International Conference on Tomography of Materials and Structures
Degree of recognition: International
Links:

Related event

3rd International Conference on Tomography of 3D Materials and Structures
26/06/2017 → 30/06/2017
Lund, Sweden
Activity: Talks and presentations › Conference presentations

Pulsed laser deposition (PLD) of the CZTS absorber for thin solar cells with up to 5.2-% -efficiency
Period: 26 Jun 2017 → 30 Jun 2017
Jørgen Schou (Guest lecturer)
Andrea Carlo Cazzaniga (Other)
Stela Canulescu (Other)
Andrea Crovetto (Other)
Rebecca Bolt Ettlinger (Other)
Nini Pryds (Guest lecturer)
Ole Hansen (Other)
Chang Yan (Other)
Kaiwen Sun (Other)
Xiaojing Hao (Other)

Department of Photonics Engineering
Optical Microsensors and Micromaterials
Department of Physics
Experimental Surface and Nanomaterials Physics
Silicon Microtechnology
Multiphase oxygen electrodes for solid oxide electrolysis cells
Period: 22 Jun 2017
Dordije Tripkovic (Speaker)
Peter Vang Hendriksen (Other)
Mogens Bjerg Mogensen (Other)
Department of Energy Conversion and Storage
Mixed Conductors

Description
Solid oxide electrolysis has the potential to become the most efficient way to convert electrical into chemical energy. Solid oxide electrolysis cells (SOEC) are thus an attractive solution for converting the occasional surplus amount of electricity produced by renewable energy sources to hydrogen or syngas. This promising technology requires further maturation to become economically competitive. Among other problems, the sluggish reaction at the oxygen electrode limits maximum fuel production rate, which directly affects overall process efficiency. Recent studies published by several groups highlight the importance of dissimilar interfaces and surface chemistry in promoting oxygen electrode reaction rate, opening a new route to enhance the electrode performance. Particularly, perovskite (113)/Ruddlesden-Popper (214) interface has been reported as highly beneficial for strontium doped lanthanum cobaltite (LSC) electrodes.[1–3]

The aim of this study is to investigate the potential of 113/214 interface to improve cobalt-free electrodes such as strontium doped lanthanum ferrite (LSF). The performance of LSF113/LSF214 couples is assessed by electrical conductivity relaxation (ECR) of geometrically well-defined electrodes, as well as by electrochemical impedance spectroscopy (EIS) of thin film electrodes prepared by PLD. The surface of the model electrodes is deliberately modified in a controlled manner by addition of secondary phases and examined by SEM and surface-sensitive characterization techniques.

Degree of recognition: International
Documents:
SSI21 abstract DJTRI
Links:
http://www.chimica.unipd.it/ssi21/ (The official conference website)
Gave a presentation on: Potential of waste heat and waste cold energy recovery in Singapore for district cooling applications
Degree of recognition: International

Related event

40th Annual IAEE International Conference
18/06/2017 → 21/06/2017
Singapore, Singapore
Activity: Talks and presentations › Conference presentations

21st International Conference on Solid State Ionics
Period: 18 Jun 2017 → 23 Jun 2017
Vincenzo Esposito (Organizer)
Department of Energy Conversion and Storage
Ceramic Engineering & Science

Description
Low-dimensional ionic and mixed ionic/electronic conductor nanostructures
Links:
http://www.chimica.unipd.it/ssi21/Symposium_II_1.html

Related event

21st International Conference on Solid State Ionics
18/06/2017 → 23/06/2017
Padova, Italy
Activity: Attending an event › Participating in or organising a conference

21st INTERNATIONAL CONFERENCE ON SOLID STATE IONICS
Period: 18 Jun 2017 → 23 Jun 2017
Didier Blanchard (Guest lecturer)
Department of Energy Conversion and Storage

Description
The International Conference on Solid State Ionics is a major event in the field, which is held every two years and attracts a world-wide audience.
Degree of recognition: International
Documents:
Abstract-Didier-Blanchard

Related event

21st International Conference on Solid State Ionics
18/06/2017 → 23/06/2017
Padova, Italy
Activity: Talks and presentations › Conference presentations

High ionic conductivity in confined heterostructures
Period: 18 Jun 2017 → 23 Jun 2017
Simone Sanna (Speaker)
Department of Energy Conversion and Storage
Electrofunctional materials

Description
High ionic conductivity in confined heterostructures

Simone Sanna (a)*, Vincenzo Esposito (a), Nini Pryds (a)
(a) Department of Energy, Technical University of Denmark, DK-4000 Roskilde, Denmark
*sime@dtu.dk
The charge transport in oxide thin films could be tuned by the lattice strain engineering resulting in a new class of materials that can be considered fundamental bricks of new generation of devices for energy storage, conversion, and information [1-5].

In particular oxide heterostructures are a very promising type of artificial materials owing to possibility to manipulate the ionic and electronic properties at the interfaces by controlling the properties of the different layers, e.g. epitaxial strain. In these heterostructures, size effects of the layers can lead to enhanced conductivity of the charge carries at the interfaces when, for example, the number of interfaces is increased and/or the thickness of the individual layers decrease.

High conductivity in thin heterostructures is often attributed either to the presence of a high density of defects, strain at the interface or space charge effects [1-2]. The latter is the case for heterostructure made of alternate layers of doped Ceria (SDC) and stabilized Zirconia (YSZ) where the ionic conductivity can increase about two order of compared to bulk [2]. However we have demonstrated that the heterostructures could be engineered in order to preserve materials with high ionic conductivity but usually, unstable by confining in more stable materials. This is the case for heterostructures based on bismuth-oxide-based materials.

Indeed 5-Bi2O3 with the fluorite structure can be confined at room temperature by depositing alternating layers of bismuth-based oxide material stacked between fluorite materials as Gadolinium-doped Ceria (CGO) or YSZ [4-5]. As consequence, the heterostructures based on bismuth-oxide remain stable without degradation under oxidizing and reducing conditions for a wide range of temperatures, and maintain the high ionic conductivity characteristic of the typical bismuth oxide.

References

Degree of recognition: International
Documents:
II-1-20170203-124311-U4CH-ORAL

Related external organisation

21st International Conference on Solid State Ionics
Padua, Italy
Activity: Talks and presentations › Conference presentations

Demonstration of Impedance Spectroscopy as a Method to Evaluate Losses of Polymer Electrolyte Membrane Electrolysis Cells during Water Electrolysis
Period: 14 Jun 2017
Katrine Elsøe (Guest lecturer)
Department of Energy Conversion and Storage

Related event

International Conference on Electrolysis
12/06/2017 → 15/06/2017
Copenhagen, Denmark
Activity: Talks and presentations › Conference presentations

Solid Oxide Electrolysis for Grid Balancing: Recent Achievements and Future Challenges
Period: 13 Jun 2017 → 15 Jun 2017
Ming Chen (Speaker)
Department of Energy Conversion and Storage

Mixed Conductors

Description
Solid oxide electrolysis is a promising technology for energy storage and synthetic fuel production and it has a unique potential for grid regulation in the Danish power system. In this presentation results from the recent ForskEL projects coordinated by DTU Energy on developing the SOEC technology were presented.

Degree of recognition: International

Related event
Alkaline membrane electrolysis with PEM-level electrochemical performance
Period: 12 Jun 2017
Mikkel Rykær Kraglund (Guest lecturer)
Department of Energy Conversion and Storage
Proton conductors
Degree of recognition: International
Documents:
ICE2017_KraglundMR_Alkaline membrane electrolysis with PEM-level electrochemical performance

Related event
International Conference on Electrolysis
12/06/2017 → 15/06/2017
Copenhagen, Denmark
Activity: Talks and presentations › Conference presentations

Development of novel High Temperature and Pressure Alkaline Electrolysis Cells (HTP-AEC)
Period: 12 Jun 2017 → 15 Jun 2017
Jens Quitzau Adolphsen (Guest lecturer)
Department of Energy Conversion and Storage
Ceramic Engineering & Science
Description
Poster presentation during the conference
Documents:
HTP-AEC Poster for ICE 2017 - JensQAdolphsen

Related event
International Conference on Electrolysis
12/06/2017 → 15/06/2017
Copenhagen, Denmark
Activity: Talks and presentations › Conference presentations

Development of novel High Temperature and Pressure Alkaline Electrolysis Cells (HTP-AEC)
Period: 12 Jun 2017 → 15 Jun 2017
Jens Quitzau Adolphsen (Speaker)
Vanessa Gil (Other)
Bhaskar Reddy Sudireddy (Other)
Christodoulos Chatzichristodoulou (Other)
Department of Energy Conversion and Storage
Ceramic Engineering & Science
Electrochemical Materials and Interfaces
Degree of recognition: International
Documents:
Registration for ICE2017-JensQAdolphsen

Related event
1st International Conference on Electrolysis
13/06/2017 → 15/06/2017
Copenhagen, Denmark
**Tutorial on high-throughput computations**  
Period: 29 May 2017 → 31 May 2017  
Simon Loftager (Participant)  
Department of Energy Conversion and Storage  
Atomic scale modelling and materials  

**Description**  
MARVEL/MaX/Psi-k tutorial on high-throughput computations: General methods and applications using AiiDA  
Degree of recognition: International  

**Related event**  
Tutorial on high-throughput computations: General methods and applications using AiiDA  
29/05/2017 → 31/05/2017  
Lausanne, Switzerland  
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

**EMRS Spring meeting 2017**  
Period: 23 May 2017  
Jørgen Schou (Participant)  
Andrea Carlo Cazzaniga (Participant)  
Stela Canulescu (Organizer)  
Rebecca Bolt Ettlinger (Participant)  
Nini Pryds (Participant)  
Ole Hansen (Organizer)  
Andrea Crovetto (Organizer)  
Chang Yan (Participant)  
Kaiwen Sun (Participant)  
Xiaojing Hao (Participant)  
Department of Photonics Engineering  
Photovoltaic Materials and Systems  
Optical Microsensors and Micromaterials  
Department of Energy Conversion and Storage  
Electrofunctional materials  
Experimental Surface and Nanomaterials Physics  
Department of Micro- and Nanotechnology  
Silicon Microtechnology  
Department of Physics  

**Description**  
Pulsed laser deposition (PLD) of the CZTS absorber for thin solar cells with up to 5.2-% -efficiency  
Degree of recognition: International  
Documents:  
Abstract Earth-abundant CZTS  

**Related event**  
EMRS Spring meeting 2017  
22/05/2017 → 26/05/2017  
Strasbourg, France  
Activity: Attending an event › Participating in or organising a conference
High ionic conductivity in confined heterostructures
Period: 27 Apr 2017
Simone Sanna (Guest lecturer)
Department of Energy Conversion and Storage
Electrofunctional materials

Description
A new class of materials that can be considered fundamental bricks of new generation of devices for energy storage, conversion, and information [1-5]. In particular oxide heterostructures are a very promising type of artificial materials owing to possibility to manipulate the ionic and electronic properties at the interfaces by controlling the properties of the different layers, e.g. epitaxial strain. In these heterostructures, size effects of the layers can lead to enhanced conductivity of the charge carries at the interfaces when, for example, the number of interfaces is increased and/or the thickness of the individual layers decrease. High conductivity in thin heterostructures is often attributed either to the presence of a high density of defects, strain at the interface or space charge effects [1-2]. The latter is the case for heterostructure made of alternate layers of doped Ceria (SDC) and stabilized Zirconia (YSZ) where the ionic conductivity can increase about two order of compared to bulk [2]. However we have demonstrated that the heterostructures could be engineered in order to preserve materials with high ionic conductivity but usually, unstable by confining in more stable materials. This is the case for heterostructures based on bismuth-oxide-based materials.
Indeed δ-Bi2O3 with the fluorite structure can be confined at room temperature by depositing alternating layers of bismuth-based oxide material stacked between fluorite materials as Gadolinium-doped Ceria (CGO) or YSZ [4-5]. As consequence, the heterostructures based on bismuth-oxide remain stable without degradation under oxidizing and reducing conditions for a wide range of temperatures, and maintain the high ionic conductivity characteristic of the typical bismuth oxide.

References

Degree of recognition: International

Documents:

Abstract_Simone Sanna
Links:
https://riuma.uma.es/xmlui/handle/10630/13505

Related external organisation

University of Malaga
Spain
Activity: Talks and presentations › Guest lectures, external teaching and course activities at other universities

Solid-state lithium sulfur batteries using nanoconfined complex hydrides as solid electrolytes
Period: 26 Apr 2017 → 27 Apr 2017
Didier Blanchard (Other)
Department of Energy Conversion and Storage

Description
Poster Presentation
Degree of recognition: International
Documents:
Li-SM3-Poster-Abstract-Blanchard

Related event

2nd Conference on Lithium Sulfur: Mechanisms, Modelling & Materials (Li-SM$^3$ 2017)
26/04/2017 → 27/04/2017
London, United Kingdom
Activity: Talks and presentations › Conference presentations

Materials Research Society Spring Meeting 2017
Period: 17 Apr 2017 → 21 Apr 2017
Jørgen Schou (Organizer)
Andrea Carlo Cazzaniga (Participant)
Andrea Crovetto (Participant)
Rebecca Bolt Ettlinger (Participant)
Sara Lena Josefin Engberg (Participant)
Stela Canulescu (Participant)
Nini Pryds (Participant)
Ole Hansen (Participant)
Chang Yan (Participant)
Kaiwen Sun (Participant)
Xiaojing Hao (Participant)
Department of Photonics Engineering
Photovoltaic Materials and Systems
Department of Physics
Experimental Surface and Nanomaterials Physics
Optical Microsensors and Micromaterials
Technical University of Denmark
Department of Energy Conversion and Storage
Electrofunctional materials
Department of Micro- and Nanotechnology
Silicon Microtechnology

**Description**
Pulsed laser deposition (PLD) of a CZTS-absorber for thin solar cells with up to 5.2% efficiency

Degree of recognition: International

Documents:
MRS 2017_poster_JS_2

**Related event**

**Materials Research Society Spring Meeting 2017**
17/04/2017 → 21/04/2017
Phoenix, United States
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

**Phosphoric Acid Anion Migration through Polybenzimidazole Membrane**

Period: 9 Apr 2017

Hans Becker (Speaker)

Department of Energy Conversion and Storage

Proton conductors

Degree of recognition: International

**Related event**

**CARISMA Conference 2017**
09/04/2017 → 12/07/2017
Newcastle, United Kingdom
Activity: Talks and presentations › Conference presentations

**Udfordringer ved VE-gas anvendt i brændselsceller**

Period: 22 Mar 2017

Anke Hagen (Guest lecturer)

Department of Energy Conversion and Storage

Applied Electrochemistry

**Description**

Invited talk

**Related event**

**IDA KEMI**
22/03/2017 → 22/03/2017
Copenhagen, Denmark
Activity: Talks and presentations › Conference presentations

**Workshop for electromechanical and dielectric materials and devices**

Period: 9 Mar 2017

Astri Bjørnetun Haugen (Organizer)
Hugh Simons (Organizer)

Department of Energy Conversion and Storage

Ceramic Engineering & Science

Department of Physics

Neutrons and X-rays for Materials Physics

Documents:
Workshop_poster
DFT Studies of the ORR Activity of Carbon Encapsulated Fe3C
Period: 1 Mar 2017
Heine Anton Hansen (Other)
Department of Energy Conversion and Storage
Atomic scale modelling and materials
Degree of recognition: International

Related event
European Fuel Cell Car Workshop
01/03/2017 → 03/03/2017
Orleans, France
Activity: Talks and presentations › Conference presentations

MODELING OF LI-ION BATTERY PACKS AS BASIS FOR DESIGN OF BATTERY THERMAL MANAGEMENT SYSTEMS
Period: 6 Feb 2017
Kurt Engelbrecht (External examiner)
Department of Energy Conversion and Storage
Electrofunctional materials

Description
External opponent on PhD thesis
Degree of recognition: National
Activity: Examinations and supervision › External examination

41st International Conference and Expo on Advanced Ceramics and Composites
Period: 22 Jan 2017 → 27 Jan 2017
Vincenzo Esposito (Organizer)
Department of Energy Conversion and Storage
Ceramic Engineering & Science

Description
14th International Symposium on Solid Oxide Fuel Cells (SOFC): Materials, Science and Technology
Links:
http://ceramics.org/icacc17-s3

Related event
41st International Conference and Expo on Advanced Ceramics and Composites
22/01/2017 → 27/01/2017
Florida, United States
Activity: Attending an event › Participating in or organising a conference

Ceramic processing of tubular, multilayered oxygen transport membranes (Invited)
Period: 22 Jan 2017 → 27 Jan 2017
Astri Bjørnetun Haugen (Invited speaker)
Department of Energy Conversion and Storage
Ceramic Engineering & Science
Pure oxygen gas supplied by ceramic oxygen transport membranes (OTMs) can facilitate reduced CO2 emissions through more efficient gasification or combustion processes and easier CO2 capture and storage. For maximum oxygen flux and 100% selectivity, the active OTM layer should be thin and dense, and have a large and catalytically activated surface area. These requirements call for an asymmetric OTM design with a thin, dense OTM layer (~15 μm) sandwiched between two porous catalyst layers (~15 μm) and mechanically supported on a porous ceramic substrate (~1 mm). This talk pertains to our work at the Technical University of Denmark (DTU) related to processing such multilayered ceramic components with a tubular geometry, focusing on scalable process technologies. This includes thermoplastic extrusion to shape the porous, tubular support, deposition of thin dense and porous layers by dip coating, co-sintering of these layers, and infiltration of electrocatalysts. Material and processing considerations for two different combinations of materials in the multilayered components will be discussed, and performance of these components under laboratory testing and integrated in pilot-scale biomass gasifiers will be presented.

Degree of recognition: International

Documents:
Abstract_ICACC217

Related event

41st International Conference and Expo on Advanced Ceramics and Composites
22/01/2017 → 27/01/2017
Florida, United States
Activity: Talks and presentations › Conference presentations

Thermo-mechanical properties of Metal-supported Solid Oxide Fuel Cells components
Period: 22 Jan 2017 → 27 Jan 2017
Francesca Teocoli (Speaker)
Department of Energy Conversion and Storage
Ceramic Engineering & Science

Description
41st Int'l Conf & Expo on Advanced Ceramics & Composites (ICACC 2017)
Degree of recognition: International

Related external organisation

The American Ceramic Society
United States
Activity: Talks and presentations › Conference presentations

Properties of multicrystalline silicon wafers and case study of PV module viability analysis
Period: 20 Jan 2017 → 16 Jun 2017
Jacob R. Bowen (Supervisor)
Marisa Di Sabatino Lundberg (Main supervisor)
Department of Energy Conversion and Storage
Imaging and Structural Analysis

Description
Degree of recognition: International
Links:
https://www.ntnu.edu/studies/msisee/solar-cellsystems-materials (Solar Cell Systems and Materials study track)
Proton conductors

Description
Ternary alkaline polybenzimidazole-based electrolytes

Related event
13/06/2016 → 16/06/2016
Zaragoza, Spain

ChemSusChem (Journal)
Period: 2016
Anke Hagen (Reviewer)
Department of Energy Conversion and Storage
Applied Electrochemistry

Related journal
ChemSusChem
1864-5631
Central database

Direct use of biogas in SOFC
Period: 2016
Anke Hagen (Other)
Department of Energy Conversion and Storage
Applied Electrochemistry

Description
Kandidatspeciale
Coordinated by Anke Hagen

ELSEVIER (Publisher)
Period: 2016
Vincenzo Esposito (Editor)
Ceramic Engineering & Science
Department of Energy Conversion and Storage

Description
Metal Oxide-Based Thin Film Structures
Degree of recognition: International
Links:
https://www.elsevier.com/books/metal-oxide-based-thin-film-structures/pryds/978-0-12-810418-7
**Journal of Industrial and Engineering Chemistry (Journal)**  
Period: 2016  
Anke Hagen (Reviewer)  
Department of Energy Conversion and Storage  
Applied Electrochemistry  

**Related journal**  
Journal of Industrial and Engineering Chemistry  
1226-086X  
Central database  
Activity: Research › Peer review of manuscripts

**Journal of Power Sources (Journal)**  
Period: 2016  
Anke Hagen (Reviewer)  
Department of Energy Conversion and Storage  
Applied Electrochemistry  

**Related journal**  
Journal of Power Sources  
0378-7753  
Central database  
Activity: Research › Peer review of manuscripts

**Kopernikus PsX (External organisation)**  
Period: 2016 → 2026  
Anke Hagen (Chairman)  
Department of Energy Conversion and Storage  
Applied Electrochemistry  

**Description**  
International Advisory Board member  

**Related external organisation**  
Kopernikus PsX  
Germany  
Activity: Membership › Membership of committees, commissions, boards, councils, associations, organisations, or similar

**PhD Thesis Kristian B. Knudsen: Censor**  
Period: 2016  
Anke Hagen (Internal examiner)  
Department of Energy Conversion and Storage  
Applied Electrochemistry  

**Description**  
Censor  
Activity: Examinations and supervision › Internal examination
Polish Science Foundation (External organisation)
Period: 2016
Anke Hagen (Chairman)
Department of Energy Conversion and Storage
Applied Electrochemistry

Description
Evaluation of proposals

Related external organisation

Polish Science Foundation
Poland
Activity: Membership › Membership in review committee

Solid State Protonic Conductors 18
Period: 2016
David Aili (Participant)
Department of Energy Conversion and Storage
Proton conductors

Description
Acid-base chemistry and proton conductivity of solid acids and their mixtures with N-heterocycles

Related event

Solid State Protonic Conductors 18
18/09/2016 → …
Oslo, Norway
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Ternary polybenzimidazole-based alkaline electrolytes
Period: 2016
David Aili (Invited speaker)
Department of Energy Conversion and Storage
Proton conductors

Related event

Workshop on Ion Exchange Membranes for Energy Applications
27/06/2016 → …
Bad Zwischenahn, Germany
Activity: Talks and presentations › Guest lectures, external teaching and course activities at other universities

Wissenschaftsfonds FWF (Fonds zur Förderung der wissenschaftlichen Forschung) Österreichs (External organisation)
Period: 2016
Anke Hagen (Chairman)
Department of Energy Conversion and Storage
Applied Electrochemistry

Description
Evaluation of proposals

Related external organisation

Wissenschaftsfonds FWF (Fonds zur Förderung der wissenschaftlichen Forschung) Österreichs
Austria  
Activity: Membership › Membership in review committee

**Integrated computational and experimental design of next-generation battery materials**  
Period: 9 Dec 2016  
Tejs Vegge (Invited speaker)  
Department of Energy Conversion and Storage  
Atomic scale modelling and materials  

**Related event**  
**SDU Energy Club**  
09/12/2016 → 09/12/2016  
Odense, Denmark  
Activity: Talks and presentations › Conference presentations

**Batterier: Status quo og i fremtiden - Fundamentale aspekter og perspektiver**  
Period: 5 Dec 2016  
Tejs Vegge (Invited speaker)  
Department of Energy Conversion and Storage  
Atomic scale modelling and materials  

**Related event**  
**ATV Energy Storage - Batteries**  
05/12/2016 → 05/12/2016  
Kgs Lyngby, Denmark  
Activity: Talks and presentations › Conference presentations

**Intermediate Temperature Proton Conductors – Why and How**  
Period: 5 Dec 2016 → 7 Dec 2016  
Qingfeng Li (Invited speaker)  
Proton conductors  
Department of Energy Conversion and Storage  
Documents:  
IT proton conductors - abstract to Workshop on Ethanol Electrooxidation 5-7 Dec 2016 Florence.pdf  

**Related event**  
**International Workshop on Ethanol Electro-Oxidation**  
05/12/2016 → 07/12/2016  
Florence, Italy  
Activity: Talks and presentations › Guest lectures, external teaching and course activities at other universities

**Nanyang Technological University**  
Period: 1 Dec 2016 → 31 Mar 2017  
Dominik Franjo Dominkovic (Visiting researcher)  
Department of Energy Conversion and Storage  
Centre for IT-Intelligent Energy Systems in Cities  

**Description**  
As a part of my stay at NTU in collaboration with Energy Research Institute at NTU, I was developing models for assessment of district cooling (DC) potential in Singapore. The work consisted of mapping the energy resources and potential DC demand, analyzing demand patterns, conducting pre-feasibility studies and evaluating the possibility of developing DC system on a large scale.  
In the second part of the project integration of DC with the energy system was assessed. Synergies between different energy sectors were detected and the potential for utilizing them was evaluated. It was found that the DC should contribute to the overall goal of reducing GHG emissions, established by the government of Singapore, as well as to
increase energy security of the country.
Results will be presented at IAEE2017 conference in Singapore in June 2017.

Links:
http://erian.ntu.edu.sg/Pages/Home.aspx

Activity: Visiting an external institution › Visiting another research institution

7th European Kesterite Workshop
Period: 17 Nov 2016 → 18 Nov 2016
Christian Rein (Participant)
Imaging and Structural Analysis
Department of Energy Conversion and Storage

Description
CZTS synthesis using deep eutectic solvents.

Related event

7th European Kesterite Workshop
16/11/2016 → 18/11/2016
Leuven, Belgium
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Solid-State Li-S Batteries based on Borohydride Solid Electrolyte
Period: 17 Nov 2016
Didier Blanchard (Invited speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related event

Materials Research Society of Korea: MRS-K 2016 Fall meeting
16/11/2016 → 18/11/2016
Gyeongju, Korea, Republic of
Activity: Talks and presentations › Conference presentations

Solid-State Li-S Batteries based on Borohydride Solid Electrolyte
Period: 16 Nov 2016
Didier Blanchard (Invited speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related event

9th International Workshop on EEWS
15/11/2016 → 16/11/2016
Daejeon, Korea, Republic of
Activity: Talks and presentations › Guest lectures, external teaching and course activities at other universities

Computational methods for accelerated DFT-based design of energy materials
Period: 8 Nov 2016
Tejs Vegge (Invited speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related event

TUM Energy Colloquium
High Performance Thermoelectric Materials and Modules for Harvesting Waste Heat
Period: 8 Nov 2016 → 12 Nov 2016
Ngo Van Nong (Invited speaker)
Department of Energy Conversion and Storage
Electrofunctional materials

Related event
The 8th International Workshop on ADVANCED MATERIALS SCIENCE AND NANOTECHNOLOGY
08/11/2016 → 12/11/2016
Activity: Talks and presentations › Conference presentations

August Wilhelm Scheer
Start date: 6 Nov 2016 → 11 Nov 2016
Tejs Vegge (Host)
Department of Energy Conversion and Storage
Atomic scale modelling and materials
Activity: Hosting a guest lecturer

Processing parameters and raw material influence on the microstructure and performance of SiC membranes for water filtration
Period: 2 Nov 2016 → 3 Nov 2016
Michela Della Negra (Lecturer)
Department of Energy Conversion and Storage
Ceramic Engineering & Science

Related event
16th Aachener membrane Kolloquium
02/11/2016 → 03/11/2016
Aachen, Germany
Activity: Talks and presentations › Conference presentations

Materials Science & Technology 2016 (MS&T16) conference
Ming Chen (Invited speaker)
Department of Energy Conversion and Storage
Mixed Conductors
Links:
http://www.matscitech.org/technical-program/fundamentals-and-characterization/

Related event
Materials Science & Technology 2016 (MS&T16) conference: Phase Stability, Diffusion Kinetics, and Their Applications (PSDK-XI) Symposium
23/10/2016 → 27/10/2016
Salt Lake City, United States
Activity: Talks and presentations › Conference presentations

From CO2 to Sustainable Fuels and Chemicals
Tejs Vegge (Invited speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

**Description**
Oral and poster presentations

**Related event**
**EU-US Frontiers of Engineering Symposium**
17/10/2016 → 19/12/2016
Helsinki, Finland
Activity: Talks and presentations › Conference presentations

**69th Annual Gaseous Electronics Conference**
Period: 10 Oct 2016
Ming Chen (Invited speaker)
Department of Energy Conversion and Storage
**Mixed Conductors**

**Related event**
**69th Annual Gaseous Electronics Conference: Session BM1: Electrification of the chemical Industry**
10/10/2016 → 10/10/2016
Bochum, Germany
Activity: Talks and presentations › Conference presentations

**Computational design of nanoalloys using DFT calculations, genetic algorithms and machine learning**
Tejs Vegge (Invited speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

**Related event**
**8th International Conference on Multiscale Materials Modeling**
09/10/2016 → 14/10/2016
Dijon, France
Activity: Talks and presentations › Conference presentations

**PRiME 2016/230th ECS Meeting**
Period: 6 Oct 2016
Yang Hu (Speaker)
Department of Energy Conversion and Storage
**Proton conductors**

**Description**
oral presentation: Probing the active site structures of iron-based ORR catalysts

2016PRiME-230th Meeting of The Electrochemical Society (ECS)

**Related event**
**PRiME 2016/230th ECS Meeting**
02/10/2016 → 07/10/2016
Honolulu, United States
Activity: Talks and presentations › Conference presentations
Denmark-China Bilateral Workshop on Energy Conversion and Storage
Ming Chen (Organizer)
Department of Energy Conversion and Storage
Mixed Conductors

Description
Denmark-China Bilateral Workshop on Energy Conversion and Storage
Links:
http://www.energy.dtu.dk/english/News/Nyhed?id=31bf51e9-f572-4e45-8a11-c3d277750ed5

Related event
Denmark-China Bilateral Workshop on Energy Conversion and Storage
03/10/2016 → 04/10/2016
Roskilde, Denmark
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Electrochemical Characterization of PEMECs Operating at Various Current Densities
Period: 2 Oct 2016
Katrine Elsøe (Guest lecturer)
Department of Energy Conversion and Storage

Related event
PRiME 2016/230th ECS Meeting
02/10/2016 → 07/10/2016
Honolulu, United States
Activity: Talks and presentations › Conference presentations

EXPERIMENTAL PROOF OF CONCEPT OF A PIEZOELECTRIC-SHAPE MEMORY ENERGY HARVESTER
Period: 2 Oct 2016 → 2 Apr 2017
Kurt Engelbrecht (Supervisor)
Department of Energy Conversion and Storage
Electrofunctional materials

Description
The aim of this work is the experimental proof of concept of an energy harvester using shape memory effect and piezoelectricity to transform input thermal power in output electricity. The practice of recovering wasted or unused energy from the environment and making it available in form of electrical charge – i.e. energy harvesting – is attracting increasing attention since it can be employed for feeding small wireless autonomous devices as a valid alternative to batteries or grid connection. As a matter of facts, traditional solutions imply continuous maintenance (e.g. batteries need to be substituted periodically) or non-economical arrangements (e.g. connecting to the grid very small devices in remote locations is not only complicated but also anti economical). Energy harvesting then addresses the problem of feeding low-power electronics and autonomous wireless sensors (requiring few mW of electricity). Since this field of research is pretty new, not much literature is available on the topic but on the other side lot of work and improvement can be done; moreover, there is not a recognized best way of doing things, then experimental activity needs to be performed to explore possible solutions.

In this work the problem of energy harvesting is addressed to considering thermal energy as available source input, to be transformed in electrical power; this is the starting point: all that comes after is the result of studies performed within this thesis. The first step is deciding which mechanism to be employed: the choice is to use shape memory effect of Ni-Ti for converting thermal power into mechanical one and then a piezoelectric actuator that receives mechanical power as an input and converts it into electricity. The reason for that is double: on one side, a research group already provided a similar device that could be used as reference and improved; on the other, Ni-Ti is the object of ongoing research due to its incredible properties and then it is due to contribute in experiments by providing another type of application for this material.

The second step is then gathering information on shape memory alloys and piezoelectric components from literature and manufacturers and designing an experimental session to provide the other pieces of information needed for the realization of this device.

Starting from shape memory effect, it is a property exhibited by certain materials that can restore the original shape of a
plastically deformed sample by simply heating it as a consequence of a crystalline phase change – called martensitic transformation. In particular, at low temperature, below the transformation starting one, the material is in martensitic phase, which is soft and can be deformed quite easily. Then, when the specimen is heated up above a transition starting temperature, it recovers its original pre-deformation shape and converts the material to its high strength – austenitic – condition. The process is reversible, meaning that the same transformation occurs while cooling, even though some hysteresis can be detected and temperature range is slightly different. If the specimen is in a constrained configuration, i.e. it cannot recover its initial shape upon heating due to zero displacement constrains, force starts growing inside it; then, it goes down while cooling. These properties are known from literature. The problem is that it is not clear how force depends on temperature and which are relevant variables affecting performance: for this reason an experimental characterization is performed. First of all, a shape memory alloy is selected, in particular Ni-Ti due to its above the average properties, even though there are also other different classes of materials showing this effect. Then a bundle of wires of Ni-Ti is tested, considering that output force depends on cold wires temperature, hot wires temperature and pre-stress, meaning force applied to the specimen at cold state, before it is heated up and actuation, i.e. force, produced. Characterization is made for a limited but still meaningful temperature values and for a wide range of pre-stress. Results show that the best operating temperatures are 5 °C as cold temperature and 55 °C as hot one, being temperature difference fixed at 50 °C. Force difference between hot and cold states increases with pre-stress almost linearly; for this reason, a pre-stress of 1000 N is selected as the one to be employed in the device during operations. Actuation provided with these parameters is expected to be 600 N.

Moving to piezoelectricity, it is the property of producing electrical charge when submitted to a certain pressure (direct piezoelectric effect), manifested by a specific class of materials. Nowadays there are many devices employing the opposite effect – inverse piezoelectricity: they receive voltage as input and produce displacement as an output; knowing the relation between displacement and voltage it is possible to provide precise control. Among these materials, the most common one is Lead Zirconate Titanate due to its marked piezoelectric effect. Working principle is as follows: when subjected to a force, there is a shifting of electrons in the crystal structure of this material, resulting in a charge; this process is reversible in a certain range of temperature, force and electric field, meaning that if force is removed the electrons go back to initial configuration and charge goes back to zero. While inverse piezoelectric effect is well known, direct one is pretty unstudied due to limited number of practical applications: for this reason a sample of Lead Zirconate Titanate needs to be tested and characterized. The goal is to find how voltage depends on force (current is expected to be very small, while voltage relevant, for this reason it is selected as variable for evaluating the performance). In the experimental session the piezoelectric actuator is then compressed at increasingly high force and voltage is measured; moreover, the effect of compression speed is investigated since it could be a relevant variable considering that a transformation in the crystal occurs. Results show that absolute value of voltage increases almost linearly with force: when compressed the actuator produces positive voltage; then if it is shortened at maximum force and gradually released to zero stress, a negative voltage builds up: for this reason it is convenient to speak about potential difference per cycle. At 600 N, which is the force provided by Ni-Ti, potential difference is expected to be between 25 V and 35 V in relation to compression speed, which slightly affects output.

Once the properties of the two main components are clear, a device employing them is designed and built. A globally zero displacement assembly is chosen: Ni-Ti wires are clamped together with the piezoelectric actuator and then subjected to temperature fluctuation, so that they produce a force that alternatively compresses and releases the piezo, finally generating in this way an electrical charge. Water is selected as heat transfer fluid and 13 wires of 5 mm length and 0.8 mm diameter of active part are disposed circularly, perpendicularly to the flow in an optimized configuration in terms of heat transfer, held in place by plastic plates and put inside a cylindrical case. A shaft then puts the active part in connection with piezoelectric actuator, well separating it from the flow since it is not waterproof.

While designing this assembly, great care is reserved to heat transfer problem and to a detailed study of how stress/strain state should evolve during operation. As regards heat transfer, both manual computation and numerical simulations are performed in order to find a configuration where water and wires exchange heat properly, i.e. efficiently, homogeneously and fast. As a matter of facts, non-homogeneous heat transfer with the wires would result in uneven shape memory effect and then in differential displacement; moreover, being the slowest phenomenon, heat transfer affects operating frequency of the whole device; for this reason it needs to be analyzed carefully. Stress/strain problem is also studied in details, cross-referencing data from both literature and experiments: it is fundamental to design the length and number of wires compatibly with stress and displacement required by piezo, which in turn depends on shape memory effect at a given temperature. In other words, it is mandatory to run a trial and error process, where there are different involved variables that need to be compatible one with the others in order to have the device working. These studies show that aforementioned configuration of 13 wires of 5 mm length and 0.8 mm diameter is a solution to this problem; even though it is not the optimized one, it should work properly for a proof of concept.

Getting back to design, there are then auxiliary elements, in particular a hydraulic circuit composed of two identical lines, one for the hot and one for the cold side, alternatively switched by means of three way valves. Water baths provide temperature control and water flow. Their goal is exchanging heat with active part of the device, providing desired temperature change at a given frequency. The other auxiliary element is the electrical circuit, aimed at collecting and measuring the charge produced by the piezo; the main components are a series of two resistors of known resistance coupled with a voltmeter for reading the voltage and a relay for switching the circuit on and off. In particular, since generated charge is very small, it is necessary first to build up a voltage across the piezo and then to discharge it across the measurement system within a certain frequency.
Finally, there is a control/data acquisition system based on LabVIEW aiming at measuring temperatures with thermocouples and recording it and at automatically switch electrical circuit with a small control current while recording voltage. Once all the parts are designed, they are built and assembled and tests are run on the apparatus. Experimental setup consists in the aforementioned components, clamped with a mechanical actuator and operating as follows. The mechanical actuator provides 1000 N of pre-stress while maintaining a zero displacement configuration; the assembly made of a cylinder containing Ni-Ti active component and a shaft for rigidly transmitting force to the piezo chip is blocked between the two plates of the mechanical actuator. Two hoses connect active chamber to hydraulic circuit while two wires connect piezo to electrical circuit. Data acquisition system completes the setup. As regards operation, several experiments are done to find best working point. Sequence of operations is as follows: pre-stress is provided while cold water is circulating, then circuit is closed to discharge voltage built up by the pre-stress and opened after that; these are preliminary actions. Then, three-way valves are switched so hot water flows and heats up the wires, which expand and actuate on the piezo, generating a voltage that can be measured after closing the circuit; the circuit is then re-opened, valves switched to cold water and then a negative voltage builds up across the piezo; electrical circuit is closed again and negative voltage measured, then it is re-opened. At this point, a new cycle begins. Data acquisition saves temperature to time and voltage to time.

These data are then elaborated employing a MATLAB script where total voltage, current, power and energy harvested per cycle are measured. Results are very positive: a potential difference of 30.73 V and a current of 2.82 mA are detected; power is 44.46 mW, while harvested energy per cycle is 0.33 mJ. An efficiency index which reports harvested energy per cycle to the mass of active part – Ni-Ti – is defined and computed: it is 2.04 mJ/g. These numbers not only prove the concept of energy harvesting, but also highlight a performance that is much better than previous devices and then can be considered as a good starting point for future developments.

In particular, an optimization process of existing device is suggested as it could improve the performance dramatically. In the following there is a list of suggestions on what could be done. First of all, an observation is mandatory: this thesis is a proof of concept, meaning that there are no requirements in terms of performance, dimensions and output of the device; when designing an energy harvester for a specific application, starting point should always be electrical requirements from the load and then design should follow up. The point is that completely different devices could be built according to the kind of application: the only element in common would be the working principle. Future developments for this specific design can be summarized as follows. First of all, from a Ni-Ti point of view it could be interesting to increase the number of wires for providing a higher actuation and a bigger pre-stress as operating condition, impossible now due to limited yield strength as failure tests show. Another improvement could be made in relation to hydraulic circuit and heat transfer: in this device operating frequency is fairly slow because the temperature of heat transfer fluid is the same as Ni-Ti desired one and valves are manual. It could be possible to design automatic valves and employ higher temperature difference so that desired temperature of Ni-Ti would be reached faster and at this point valves would switch automatically. As a result, system would operate with higher frequency and then also global harvested energy would be bigger, due to more cycles in the same time interval. Finally, a wider characterization of temperature influence on Ni-Ti displacement could lead to the definition of better working conditions.

Degree of recognition: International
Documents:
2017_04_Bazzan
Activity: Examinations and supervision › Supervisor activities

Genetic Algorithms and DFT for Accelerated Design of Nanoalloys
Heine Anton Hansen (Invited speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials
Theoretical Atomic-scale Physics

Related event
PRIME 2016/230th ECS Meeting
02/10/2016 → 07/10/2016
Honolulu, United States
Activity: Talks and presentations › Conference presentations

PRiME 2016/230th ECS Meeting
Period: 2 Oct 2016
Salvatore De Angelis (Participant)
Department of Energy Conversion and Storage
Imaging and Structural Analysis

Description
Electrochemical society meeting. Oral presentation

Related event

PRiME 2016/230th ECS Meeting
02/10/2016 → 07/10/2016
Honolulu, United States
Activity: Attending an event › Participating in or organising a conference

In situ X-ray diffraction studies of electrode materials in working metal-ion batteries and other layered materials
Period: 20 Sep 2016
Rune E. Johnsen (Invited speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials
Imaging and Structural Analysis

Description
Seminar talk at Physics Department, Technical University of Munich

Related external organisation

Unknown external organisation
Activity: Talks and presentations › Conference presentations

Error Identification in DFT for Sustainable Energy Technologies
Period: 15 Sep 2016
Rune Christensen (Invited speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Description
Seminar talk at Brown University

Related external organisation

Unknown external organisation
Activity: Talks and presentations › Conference presentations

7th International Conference on Magnetic Refrigeration at Room Temperature (Thermag VII)
Period: 11 Sep 2016 → 14 Sep 2016
Christian Bahl (Speaker)
Department of Energy Conversion and Storage
Electrofunctional materials

Related event

7th International Conference on Magnetic Refrigeration at Room Temperature (Thermag VII)
Turin, Italy
Activity: Talks and presentations › Conference presentations

Brown University
Period: 11 Sep 2016 → 18 Sep 2016
Rune Christensen (Visiting researcher)
Department of Energy Conversion and Storage

Atomic scale modelling and materials

Description
Visit at Brown University: Catalyst Design Lab
Activity: Visiting an external institution › Visiting another research institution

11th Conference on Sustainable Development of Energy, Water and Environment Systems
Period: 4 Sep 2016 → 9 Sep 2016
Dominik Franjo Dominkovic (Speaker)
Department of Energy Conversion and Storage

Centre for IT-Intelligent Energy Systems in Cities

Description
Attended the conference and hold a presentation on "Improving the Performance of District Heating Systems by Utilization of Local Heat Boosters"
Degree of recognition: International
Links:
http://www.lisbon2016.sdewes.org/

Related event
11th Conference on Sustainable Development of Energy, Water and Environment Systems
04/09/2016 → 09/09/2016
Lisbon, Portugal
Activity: Talks and presentations › Conference presentations

Quasi-Elastic Neutron Scattering studies for Material Research
Period: 2 Sep 2016
Didier Blanchard (Invited speaker)
Department of Energy Conversion and Storage

Atomic scale modelling and materials

Related event
50 Years of Neutron Backscattering
02/09/2015 → 03/12/2016
Munich, Germany
Activity: Talks and presentations › Conference presentations

Dänemark ohne fossile Brennstoffe: Möglichkeiten für die Hochtemperaturbrennstoffzelle und Elektrolyse
Period: Aug 2016
Anke Hagen (Guest lecturer)
Department of Energy Conversion and Storage
Applied Electrochemistry

Description
Invited talk

Related event
Kopernikus P2X Kolloquium
24/10/2016 → 25/10/2016
Jülich, Germany
Activity: Talks and presentations › Conference presentations
SOFC/SOEC in Dänemark – Status und Herausforderungen in einer neuen Finanzierungslandschaft
Period: Aug 2016
Anke Hagen (Guest lecturer)
Department of Energy Conversion and Storage
Applied Electrochemistry

Description
Invited talk

Related event
DACH 4 SOFC/SOEC Treffen
17/10/2016 → 18/10/2016
Jülich, Germany
Activity: Talks and presentations › Conference presentations

Quasi-Elastic Neutron Scattering Studies on Solid Electrolytes for all-solid-state Lithium Batteries
Period: 30 Aug 2016
Didier Blanchard (Invited speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related event
European Crystallographic Meeting 2016
28/08/2016 → 01/09/2016
Basel, Switzerland
Activity: Talks and presentations › Conference presentations

IN-SITU TRANSMISSION ELECTRON MICROSCOPY ON OPERATING ELECTROCHEMICAL CELLS
Fabrizio Gualandris (Speaker)
Department of Energy Conversion and Storage
Imaging and Structural Analysis

Description
Partecipation at The European Microscopy Congress (EMC) 2016 with a talk. EMC is an international conference of the highest quality sitting alongside Europe's largest exhibition dedicated to microscopy. In addition to the conference and exhibition there will be great training opportunities, a programme of technical workshops, and a full social programme.
Degree of recognition: International
Documents:
Abstract
Links:
http://emc-proceedings.com/abstract/in-situ-transmission-electron-microscopy-on-operating-electrochemical-cells/
(Abstract)

Related organisation
IN-SITU TRANSMISSION ELECTRON MICROSCOPY ON OPERATING ELECTROCHEMICAL CELLS
Gualandris, F. (Speaker)
28 Aug 2016 → 2 Sep 2016
Activity: Talks and presentations › Conference presentations

SOCs for various occasions
Period: 24 Aug 2016
Søren Linderoth (Lecturer)
Department of Energy Conversion and Storage
Related event

**International Congress on Ceramics (ICC6)**
21/08/2016 → 25/08/2016
Dresden, Germany
Activity: Talks and presentations › Conference presentations

**67th Annual Meeting of the International Society of Electrochemistry in The Hague**
Heine Anton Hansen (Speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials
Theoretical Atomic-scale Physics

**Description**

Related event

**67th Annual Meeting of the International Society of Electrochemistry: Electrochemistry: from Sense to Sustainability**
21/08/2016 → 26/08/2016
The Hague, Netherlands
Activity: Talks and presentations › Conference presentations

**2016 CAMD Summer School on Electronic Structure Theory and Materials Design**
Tejs Vegge (Organizer)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

**Description**
Electrochemical Energy Conversion and Storage
co-organizer and speaker

Related event

**2016 CAMD Summer School on Electronic Structure Theory and Materials Design**
14/08/2016 → 19/08/2016
Kgs. Lyngby, Denmark
Activity: Attending an event › Participating in or organising a conference

**Atomic Scale Modeling of Electrocatalytic Reactions**
Period: 12 Aug 2016
Heine Anton Hansen (Invited speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials
Theoretical Atomic-scale Physics

**Description**
Seminar titled "Atomic Scale Modeling of Electrocatalytic Reactions" at the Scott Institute, Carnegie Mellon University, Pittsburgh.

Related event

**Atomic Scale Modeling of Electrocatalytic Reactions**
15th International Symposium on Metal-Hydrogen Systems

Period: 10 Aug 2016
Didier Blanchard (Speaker)
Department of Energy Conversion and Storage

Atomic scale modelling and materials

Description
Complex Hydrides as room-temperature solid electrolytes for rechargeable batteries

Oral Presentation

Related event

15th International Symposium on Metal-Hydrogen Systems
07/08/2016 → 12/08/2016
Interlaken, Switzerland
Activity: Talks and presentations › Conference presentations

Computational Design of Materials for Hydrogen Storage, Batteries and Electrocatalysis

Tejs Vegge (Invited speaker)
Department of Energy Conversion and Storage

Atomic scale modelling and materials

Related event

15th International Symposium on Metal-Hydrogen Systems
07/08/2016 → 12/08/2016
Interlaken, Switzerland
Activity: Talks and presentations › Conference presentations

Summer school on Smart Energy Systems and Entrepreneurship

Dominik Franjo Dominkovic (Speaker)
Department of Energy Conversion and Storage
Centre for IT-Intelligent Energy Systems in Cities

Description
Participated in and gave a pitch on "Bioliq" start-up.

Participated in and presented a pitch at the Summer school on Smart Energy Systems and Entrepreneurship organized by EIT digital and Karlsruhe Institute of Technology, Karlsruhe, Germany

Related event

Summer school on Smart Energy Systems and Entrepreneurship
25/07/2016 → 05/08/2016
Karlsruhe, Germany
Activity: Talks and presentations › Conference presentations

Bayesian statistics to improve accuracy through identification and correction of systematic errors in DFT

Tejs Vegge (Invited speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related event

TRSC: Interfacial Chemistry and Charge Transfer for Energy Storage and Conversion
25/07/2016 → 29/07/2016
Colorado, United States
Activity: Talks and presentations › Conference presentations

CEA-TUM Summer School on the Future of a Common European Strategy
Period: 6 Jul 2016
Dominik Franjo Dominkovic (Speaker)
Department of Energy Conversion and Storage
Centre for IT-Intelligent Energy Systems in Cities

Description
Participated in a summer school and presented a poster during both poster and rapid fire sessions.

Participated and presented a poster at the CEA-TUM Summer School on the Future of a Common European Strategy at Abtei Frauenwörth, Bavaria, Germany

Related event

CEA-TUM Summer School on the Future of a Common European Strategy
05/07/2016 → 10/07/2016
Chiemsee, Germany
Activity: Talks and presentations › Conference presentations

Presentation of DTU Energy: by Professor Søren Linderoth
Period: 6 Jul 2016
Søren Linderoth (Speaker)
Department of Energy Conversion and Storage
Activity: Other

12th European SOFC & SOE Forum 2016
Period: 5 Jul 2016 → 8 Jul 2016
Ming Chen (Speaker)
Department of Energy Conversion and Storage
Mixed Conductors

Related event

12th European SOFC & SOE Forum
05/07/2016 → 08/07/2016
Lucerne, Switzerland
Activity: Talks and presentations › Conference presentations

Workshop on Ion Exchange Membranes for Energy Applications
Andreas Kirkebæk (Participant)
Department of Energy Conversion and Storage
Proton conductors

Description
Comparative Study of the Effect of Various Cross Linkers upon Membrane Properties

Poster presentation
Documents:
EMEA2016 Poster - Andreas Kirkebæk

Related event

Workshop on Ion Exchange Membranes for Energy Applications
27/06/2016 → …
Bad Zwischenahn, Germany
Activity: Attending an event › Participating in or organising a conference

29th International Conference on Efficiency, Cost, Optimisation, Simulation and Environmental Impact of Energy Systems
Period: 21 Jun 2016
Dominik Franjo Dominkovic (Speaker)
Department of Energy Conversion and Storage
Centre for IT-Intelligent Energy Systems in Cities

Description
Gave a presentation on: "Benefits of Integrating Geographically Distributed District Heating Systems"

ECOS 29th International Conference
Documents:
Dominkovic_Benefits of Integrating Geographically Distributed District Heating Systems_presentation

Related event

29th International Conference on Efficiency, Cost, Optimisation, Simulation and Environmental Impact of Energy Systems
19/06/2016 → 23/08/2016
Portorož, Slovenia
Activity: Talks and presentations › Conference presentations

Computational Design of Materials for Electrochemical Energy Storage at DTU Energy
Tejs Vegge (Invited speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related event

1st Lancaster University-DTU Electrochemistry Workshop
21/06/2016 → 22/12/2016
Lancaster, United Kingdom
Activity: Talks and presentations › Conference presentations

Trends and frontiers in solid state energy conversion - materials and technologies
Period: 20 Jun 2016
Christian Bahl (Keynote speaker)
Department of Energy Conversion and Storage
Electrofunctional materials

Description
Energy conversion using solid state materials allows for simple and compact devices that can be used in energy applications. A range of materials exist which can be used for such solid state energy conversion. The best known ones are maybe the thermoelectric materials that can generate electricity from a temperature span or vice versa. The so-called caloric materials will change their temperature when exposed to an external field, which may be magnetic, electrical or mechanical. These can be used either for heat pumping, or for generating energy from waste heat. The available materials for solid state energy conversion technologies will be reviewed and the present state of the art of these technologies will be discussed.

Related event
6th Baltic Electrochemistry Conference
Period: 17 Jun 2016
Marko Melander (Speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

**Description**
Participation and presentation at the 6th Baltic Electrochemistry Conference

**Related event**
6th Baltic Electrochemistry Conference
15/06/2016 → 17/06/2016
Helsinki, Finland
Activity: Talks and presentations › Conference presentations

2nd South East European Conference on Sustainable Development of Energy, Water and Environment Systems
Dominik Franjo Dominkovic (Speaker)
Department of Energy Conversion and Storage
Centre for IT-Intelligent Energy Systems in Cities

**Description**
I gave a presentation on: "Modelling transition towards sustainable transportation sector". I was coauthor of two additional papers that were presented during the conference.

2nd South East European Conference on Sustainable Development of Energy, Water and Environment Systems
Documents:
Dominkovic_Modelling transition towards sustainable transportation sector

**Related event**
2nd South East European Conference on Sustainable Development of Energy, Water and Environment Systems
15/06/2016 → 18/06/2016
Piran, Slovenia
Activity: Talks and presentations › Conference presentations

Nanoconfined LiBH4 in mesoporous silica scaffold as solid electrolyte for solid-state Lithium battery
Period: 14 Jun 2016
Didier Blanchard (Invited speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

**Related event**
EMN Meeting on mesoporous materials: EMN
13/06/2016 → 17/06/2016
Prague, Czech Republic
Activity: Talks and presentations › Conference presentations

Hydrogen2Storage & Transport in Denmark
Period: 8 Jun 2016
Ming Chen (Participant)
Department of Energy Conversion and Storage

Mixed Conductors

Related event

Hydrogen²Storage & Transport in Denmark
08/06/2016 → 08/06/2016
Copenhagen, Denmark
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

GPAW 2016: Users and developers meeting
Marko Melander (Speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials
Description
GPAW developers meeting

Related event

GPAW 2016: Users and developers meeting
06/06/2016 → 10/06/2016
Jyväskylä, Finland
Activity: Talks and presentations › Conference presentations

Effect of fast mass diffusion regime on defective ceria mechano-chemo-electrical properties: By Vincenzo Esposito
Period: 2 Jun 2016
Vincenzo Esposito (Invited speaker)
Department of Energy Conversion and Storage
Ceramic Engineering & Science
Description
Invited Talk - Mechano-Electro-Chemical Coupling in Energy Related Materials and Devices 2 symposium at the 229th ECS mtg.
Links:
http://ma.ecsdl.org/content/MA2016-01/30/1496.abstract

Related event

The 229th ECS Meeting
29/05/2016 → 02/06/2016
San Diego, CA, United States
Activity: Talks and presentations › Conference presentations

Hydrides as Energy Materials
Period: 2 Jun 2016
Didier Blanchard (Speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials
Description
Solid-State Lithium-Sulfur Batteries Based on Nano-Confined LiBH₄
Oral Presentation

Related event
Integrated Computational and Experimental Design of Next-Generation Battery Materials
Period: 1 Jun 2016 → 3 Jun 2016
Tejs Vegge (Invited speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related event
01/06/2016 → 03/06/2016
Aarhus, Denmark
Activity: Talks and presentations › Conference presentations

The 229th ECS Meeting
Period: 29 May 2016 → 2 Jun 2016
Heine Anton Hansen (Speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials
Theoretical Atomic-scale Physics

Description
Oral talk: "ORR Activity of Pristine Graphite|Fe3c Interfaces"

Related event
The 229th ECS Meeting
29/05/2016 → 02/06/2016
San Diego, CA, United States
Activity: Talks and presentations › Conference presentations

The 229th ECS Meeting
Period: 29 May 2016 → 2 Jun 2016
Vladimir Tripkovic (Speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials
Theoretical Atomic-scale Physics

Description
Tailoring the performance of oxides for the oxygen evolution reaction

Related event
The 229th ECS Meeting
29/05/2016 → 02/06/2016
San Diego, CA, United States
Activity: Talks and presentations › Conference presentations

Lithium-Sulfur Solid-State Batteries Based on Nanoconfined LiBH4
Period: 24 May 2016
Didier Blanchard (Invited speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related event

2nd Cracow’s meeting on concepts related to energy
24/05/2016 → 25/05/2017
Cracow, Poland
Activity: Talks and presentations › Conference presentations

9th European Heat Pump Forum
Period: 18 May 2016 → 20 May 2016
Dominik Franjo Dominkovic (Participant)
Department of Energy Conversion and Storage
Centre for IT-Intelligent Energy Systems in Cities

Description
Participated in the 9th EHPA forum held in Paris, France.

9th European Heat Pump Forum

Related event

9th European Heat Pump Forum
18/08/2016 → 20/08/2016
Paris, France
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

2016 E-MRS Spring Meeting and Exhibit
Period: 2 May 2016 → 6 May 2016
Rune E. Johnsen (Speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials
Imaging and Structural Analysis

Description
Title: Micro-battery cells for detailed in situ X-ray diffraction studies of electrode materials in working metal-ion batteries

Related event

2016 E-MRS Spring Meeting and Exhibit
02/05/2016 → 06/05/2016
Lille, France
Activity: Talks and presentations › Conference presentations

Solid Oxide Fuel Cells at DTU Energy – From fundamental research towards application for renewable energy systems
Period: Apr 2016
Anke Hagen (Guest lecturer)
Department of Energy Conversion and Storage
Applied Electrochemistry

Related event

Sino-Denmark Bilateral Forum: Possibilities and Challenges of Solid Oxide Cells in Energy Transition
08/04/2016 → 11/04/2016
Shanghai, China
Activity: Talks and presentations › Conference presentations
Large scale heat pumps as a link between intermittent electrical energy sources and district heating sector
Period: 20 Apr 2016
Dominik Franjo Dominkovic (Invited speaker)
Department of Energy Conversion and Storage
Centre for IT-Intelligent Energy Systems in Cities

Related event

22nd International Trade Fair and Congress for Heating, Cooling and CHP
19/04/2016 → 21/06/2016
Frankfurt/Main, Germany
Activity: Talks and presentations › Conference presentations

Introduction to DTU Energy Research
Period: 8 Apr 2016
Søren Linderoth (Participant)
Department of Energy Conversion and Storage

Description
DTU Visit - SICCAS and SINAP/China, about SOFC research

Related event

Introduction to DTU Energy Research
08/04/2016 → 08/04/2016
Shanghai, China
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Sino-Denmark Bilateral Forum: Possibilities and Challenges of Solid Oxide Cells in Energy Transition
Period: 8 Apr 2016 → 11 Apr 2016
Søren Linderoth (Speaker)
Department of Energy Conversion and Storage

Description
Energy Conversion Technology Development at DTU Energy

Related event

Sino-Denmark Bilateral Forum: Possibilities and Challenges of Solid Oxide Cells in Energy Transition
08/04/2016 → 11/04/2016
Jiangsu, China
Activity: Talks and presentations › Conference presentations

Sino-Denmark Bilateral Forum: Possibilities and Challenges of Solid Oxide Cells in Energy Transition
Period: 8 Apr 2016 → 11 Apr 2016
Ming Chen (Organizer)
Department of Energy Conversion and Storage
Mixed Conductors

Description
Chairman
Links:
http://www.energy.dtu.dk/english/News/Nyhed?id=d4f4b6e9-6e62-42b0-aacf-87c29a1ad8da

Related event

Sino-Denmark Bilateral Forum: Possibilities and Challenges of Solid Oxide Cells in Energy Transition
08/04/2016 → 11/04/2016
Shanghai, China
Hydrogen Day 2016
Period: 6 Apr 2016 → 8 Apr 2016
Qingfeng Li (Participant)
Department of Energy Conversion and Storage
Proton conductors

Description
Invited talk
Documents:
Abstract CISTEM Symposium 6-8 April 2016, Prague

Related event
Hydrogen Day 2016: 7th International Conference on Hydrogen Technologies
06/04/2016 → 08/04/2016
Prague, Czech Republic
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Computational Design of Materials Atomic-scale modeling of electrode reactions in Zn-air batteries
Period: 4 Apr 2016 → 6 Apr 2016
Tejs Vegge (Invited speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related event
1st International Zinc-Air Battery Workshop
04/04/2016 → 06/04/2016
Ulm, Germany
Activity: Talks and presentations › Conference presentations

Challenges in Going from 2nd Order to 1st Order Materials in Magnetic Refrigeration Devices
Period: 28 Mar 2016 → 1 Apr 2016
Christian Bahl (Invited speaker)
Department of Energy Conversion and Storage
Electrofunctional materials

Related event
2016 MRS Spring Meeting
28/03/2016 → 01/04/2016
Phoenix, United States
Activity: Talks and presentations › Conference presentations

Electrolysis and electrochemistry
Anke Hagen (Other)
Department of Energy Conversion and Storage
Applied Electrochemistry

Related event
Interdisciplinary Block Course „Energy and Chemistry“
29/02/2016 → 04/03/2016
Karlsruhe, Germany
Boron removal from molten silicon using different gas blowing mixtures
Period: 26 Feb 2016 → 26 Jul 2016
Jacob R. Bowen (Supervisor)
Gabriella Tranell (Main supervisor)
Jafar Safarian (Supervisor)
Department of Energy Conversion and Storage
Imaging and Structural Analysis

Description
Degree of recognition: International
Activity: Examinations and supervision » Supervisor activities

10th International Symposium "Hydrogen & Energy"
Period: 21 Feb 2016 → 26 Feb 2016
Didier Blanchard (Speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Description
LITHIUM-SULFUR ALL-SOLID-STATE BATTERIES
Oral presentation

Related event
10th International Symposium "Hydrogen & Energy"
21/02/2016 → 26/02/2016
Sendai, Japan
Activity: Talks and presentations » Conference presentations

Computational Design of Materials for Electrochemical Energy Conversion and Storage
Tejs Vegge (Invited speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related event
10th International Symposium "Hydrogen & Energy"
21/02/2016 → 26/02/2016
Sendai, Japan
Activity: Talks and presentations » Conference presentations

Platform for smart energi, Energistyrelsen (External organisation)
Period: 15 Feb 2016 → 30 Jun 2017
Allan Schrøder Pedersen (Participant)
Department of Energy Conversion and Storage
Centre for IT-Intelligent Energy Systems in Cities

Related external organisation
Platform for smart energi, Energistyrelsen
Activity: Membership » Membership of commitees, commissions, boards, councils, associations, organisations, or similar
40th International Conference and Exposition on Advanced Ceramics and Composites  
Period: 24 Jan 2016 → 29 Jan 2016  
Vincenzo Esposito (Organizer)  
Department of Energy Conversion and Storage  
Ceramic Engineering & Science  

**Description**  
13th International Symposium on Solid Oxide Fuel Cells (SOFC): Materials, Science, and Technology  

13th International Symposium on Solid Oxide Fuel Cells (SOFC): Materials, Science, and Technology  
Links:  

**Related event**  
40th International Conference and Exposition on Advanced Ceramics and Composites: ICACC´16  
24/01/2016 → 29/01/2016  
Daytona Beach, FL, United States  
Activity: Attending an event › Participating in or organising a conference  

---

**High Pressure Synthesis of Non-precious Metal ORR Catalysts for Fuel Cells**  
Period: 18 Jan 2016 → 19 Jan 2016  
Qingfeng Li (Invited speaker)  
Department of Energy Conversion and Storage  
Proton conductors  

**Description**  
Invited speaker  
Documents:  
Abstract on NPMC submitted to 1st Curtin-UQ Workshop 18-19 Jan 2016  

**Related event**  
Curtin - University of Queensland Workshop on Nanostructured Electromaterials for Energy  
18/01/2016 → 19/01/2016  
Perth, Australia  
Activity: Talks and presentations › Guest lectures, external teaching and course activities at other universities  

---

24th International Materials Research Congress  
Period: 2015  
Henrique Neves Bez (Speaker)  
Department of Energy Conversion and Storage  
Electrofunctional materials  

**Related event**  
24th International Materials Research Congress  
16/08/2015 → 20/08/2015  
Cancun, Mexico  
Activity: Talks and presentations › Conference presentations  

---

Annual Meeting of the Danish Electrochemical Society 2015  
Period: 2015  
Yang Hu (Speaker)  
Department of Energy Conversion and Storage
Proton conductors

**Description**
Encapsulation structure for oxygen reduction: a preliminary understanding

**Annual Meeting of the Danish Electrochemical Society 2015**

**Related event**

**Annual Meeting of the Danish Electrochemical Society 2015**
01/10/2015 → 02/10/2015
Copenhagen, Denmark
Activity: Talks and presentations › Conference presentations

**Chemical Engineering Journal (Journal)**
Period: 2015
Anke Hagen (Reviewer)
Department of Energy Conversion and Storage
Applied Electrochemistry

**Related journal**

**Chemical Engineering Journal**
1385-8947
Central database
Activity: Research › Peer review of manuscripts

**Delft Days on Magnetocalorics 2015**
Period: 2015
Henrique Neves Bez (Participant)
Department of Energy Conversion and Storage
Electrofunctional materials

**Description**
Poster presentation

**Related event**

**Delft Days on Magnetocalorics 2015**
02/11/2015 → …
Delft, Netherlands
Activity: Attending an event › Participating in or organising a conference

**European School of Magnetism**
Period: 2015 → …
Henrique Neves Bez (Participant)
Department of Energy Conversion and Storage

**Description**
From fundamental magnetism to spin currents

**Related event**

**European School of Magnetism**
24/08/2015 → 04/09/2015
Cluj-Napoca, Romania
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.
Fuel Cells (Journal)
Period: 2015
Anke Hagen (Reviewer)
Department of Energy Conversion and Storage
Applied Electrochemistry
Links:

Related journal
Fuel Cells
1615-6846
BFI (2018): BFI-level 1, Scopus rating (2017): CiteScore 1.88 SJR 0.559 SNIP 0.748, ISI indexed (2013): ISI indexed yes, Web of Science (2018): Indexed yes
Central database
Activity: Communication › Journal editor

Journal of Power Sources (Journal)
Period: 2015
Anke Hagen (Reviewer)
Department of Energy Conversion and Storage
Applied Electrochemistry
Related journal
Journal of Power Sources

International Journal of Hydrogen Energy (Journal)
Period: 2015
Anke Hagen (Reviewer)
Department of Energy Conversion and Storage
Applied Electrochemistry
Related journal
International Journal of Hydrogen Energy
0360-3199
Central database
Activity: Research › Peer review of manuscripts
Journal of Solid State Electrochemistry (Journal)
Period: 2015
Anke Hagen (Reviewer)
Department of Energy Conversion and Storage
Applied Electrochemistry
Related journal
Journal of Solid State Electrochemistry
1432-8488
BFI (2018): BFI-level 1, Scopus rating (2017): CiteScore 2.37 SJR 0.661 SNIP 0.674, ISI indexed (2013): ISI indexed yes,
Web of Science (2018): Indexed yes
Central database
Activity: Research › Peer review of manuscripts

PhD thesis Lisa Deleebeeck: Censor
Period: 2015
Anke Hagen (Internal examiner)
Department of Energy Conversion and Storage
Applied Electrochemistry
Description
Censor
Activity: Examinations and supervision › Internal examination

PhD thesis Olivier Thomann: Censor
Period: 2015
Anke Hagen (External examiner)
Department of Energy Conversion and Storage
Applied Electrochemistry
Activity: Examinations and supervision › External examination

RFCcontrol: Open source control software for fuel cell and electrolyser test stations
Period: 2015
Søren Koch (Participant)
Department of Energy Conversion and Storage
Applied Electrochemistry
Description
RFCcontrol is a generalized control system for fuel cell, electrolyser cells, battery and other types of materials test stations / test setups. It features data logging as well as device control and can handle gas flow control, temperature control, relay control, control of DC power supplies as well as handle data acquisition through a number of data logging devices.
Head: Søren Koch
Links:
http://www.rfccontrol.dk/
Related external organisation
Department of Energy Conversion and Storage
Roskilde, Denmark
Activity: Other
Study of mesoporous ZSM-5
Period: 2015 → 2016
Anke Hagen (Other)
Department of Energy Conversion and Storage
Applied Electrochemistry

Description
Diplomingenierprojekt
Coordinated by Anke Hagen

Related external organisation

DTU Energy
Roskilde, Denmark
Activity: Other

Topics in catalysis (Journal)
Period: 2015
Anke Hagen (Reviewer)
Department of Energy Conversion and Storage
Applied Electrochemistry

Related journal

Topics in catalysis
1022-5528
BFI (2018): BFI-level 1, Scopus rating (2017): CiteScore 2.57 SJR 0.965 SNIP 0.753, ISI indexed (2013): ISI indexed yes,
Web of Science (2018): Indexed yes
Central database
Activity: Research › Peer review of manuscripts

Helmholtz Institute Ulm (External organisation)
Period: 18 Dec 2015 → …
Tejs Vegge (Participant)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Description
Member of the International Advisory Board for Electrochemical Energy Storage, SCI Program, The Helmholtz Association
Member of the International Advisory Board for Electrochemical Energy Storage under the Program 'Storage and Cross-linked Infrastructure (SCI)'. SCI coordinates activities within at five different Helmholtz Centers, i.e. KIT, FZJ, DLR, HZB and HZDR. The topic Electrochemical Energy Storage covers the activities within electrochemical energy storage.

Body type: Advisory Board
Degree of recognition: International

Related external organisation

Helmholtz Institute Ulm
Germany
Activity: Membership › Membership of committees, commissions, boards, councils, associations, organisations, or similar

Accelerated DFT-based Design of Materials for Ammonia Storage
Period: 15 Dec 2015
Tejs Vegge (Invited speaker)
Related event

PacificChem 2015
15/12/2015 → 20/12/2015
Honolulu, Hawaii, United States
Activity: Talks and presentations › Conference presentations

Nordic Battery Conference 2015
Period: 2 Dec 2015 → 3 Dec 2016
Simon Loftager (Participant)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Description
The Nordic Battery Conference 2015 (NordBatt 2)

Related event

Nordic Battery Conference 2015
02/12/2015 → 03/12/2015
Trondheim, Norway
Activity: Attending an event › Participating in or organising a conference

Modelling, optimisation, design and analysis of integrated energy systems
Period: 30 Nov 2015 → 4 Dec 2015
Dominik Franjo Dominkovic (Participant)
Department of Energy Conversion and Storage
Centre for IT-Intelligent Energy Systems in Cities

Description
Successfully participated in a PhD course.

"Modelling, optimisation, design and analysis of integrated energy systems" organized by EPFL, Sion, Switzerland

Related event

Modelling, optimisation, design and analysis of integrated energy systems
30/11/2015 → 04/12/2015
Sion, Switzerland
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Computational Design of Materials for Energy Conversion and Storage
Period: 20 Nov 2015
Tejs Vegge (Invited speaker)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related event

20/11/2015 → …
Reykjavik, Iceland
Activity: Talks and presentations › Conference presentations

**Gas network modelling: Master Thesis by Marco Cavana**
Period: 15 Nov 2015 → 10 Jul 2016
Allan Schrøder Pedersen (Supervisor)
Centre for IT-Intelligent Energy Systems in Cities
Department of Energy Conversion and Storage
Activity: Examinations and supervision › Supervisor activities

**On the Analysis of Positron Lifetime Spectra**
Period: 12 Nov 2015 → 13 Nov 2015
Morten Mostgaard Eldrup (Lecturer)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

**Description**
Invited talk

Co-authors: Peter Kirkegaard and Jens V. Olsen, AIT, DTU

**Related event**

**Tagung deutscher Positronengruppen-3**
12/11/2015 → 13/11/2015
München, Denmark
Activity: Talks and presentations › Conference presentations

**DFT Studies of the Oxygen Reduction Reaction on Fe3C-graphite catalysts**
Period: 10 Nov 2015
Heine Anton Hansen (Keynote speaker)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials

**Related event**

**International Conference on Innovative Electrochemical Energy Materials and Technologies 2015**
08/11/2015 → 11/11/2015
Nanning, China
Activity: Talks and presentations › Conference presentations

**International Conference on Innovative Electrochemical Energy Materials and Technologies**
Period: 8 Nov 2015 → 11 Nov 2015
Mateusz Krzysztof Reda (Speaker)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials

**Description**
Poster presentation


**Related event**
08/11/2015 → 11/11/2015
Nanning, China
Activity: Talks and presentations › Conference presentations

International Conference on Innovative Electrochemical Energy Materials and Technologies
Period: 8 Nov 2015 → 11 Nov 2015
Mateusz Krzysztof Reda (Speaker)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Description
Co-author of oral presentation


Related event
08/11/2015 → 11/11/2015
Nanning, China
Activity: Talks and presentations › Conference presentations

A Perspective on Next-generation Battery Technologies
Period: 5 Nov 2015
Tejs Vegge (Invited speaker)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related event
Workshop on Batteries as a Game Changer?!, Intelligent Energy
05/11/2015 → …
Copenhagen, Denmark
Activity: Talks and presentations › Conference presentations

Delft Days on Magnetocalorics 2015
Period: 2 Nov 2015 → 3 Nov 2015
Christian Bahl (Participant)
Department of Energy Conversion and Storage
Electrofunctional materials

Related event
Delft Days on Magnetocalorics 2015
02/11/2015 → …
Delft, Netherlands
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Delft Days on Magnetocalorics 2015
Period: 2 Nov 2015 → 3 Nov 2015
Andrea Roberto Insinga (Participant)
Department of Energy Conversion and Storage
Electrofunctional materials

Related event

**Delft Days on Magnetocalorics 2015**
02/11/2015 → …
Delft, Netherlands
Activity: Attending an event › Participating in or organising a conference

**Danish Electrochemical Society (External organisation)**
Period: 1 Nov 2015 → …
Marie Lund Traulsen (Chairman)
Department of Energy Conversion and Storage

**Description**
Boardmember of the Danish Electrochemical Society
Degree of recognition: National
Links:
http://www.electrochemistry.dk/

**Related external organisation**

**Danish Electrochemical Society**
Munkebjergvej 17, 4100, Ringsted, Denmark
Activity: Membership › Board duties in companies, associations, or public organisations

**Descriptor based Design of Catalytic Nanoalloys and Clusters using Density Functional Theory and Genetic Algorithms**
Tejs Vegge (Invited speaker)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials

**Related event**

**International Symposium on Clusters and Nanomaterials**
26/10/2015 → 29/10/2015
Virginia, United States
Activity: Talks and presentations › Conference presentations

**High Performance Segmented Oxides-based Materials**
Ngo Van Nong (Invited speaker)
Department of Energy Conversion and Storage
Electrofunctional materials

**Related event**

*14th International Union of Materials Research Societies - International Conference on Advanced Materials*
25/10/2015 → …
Activity: Talks and presentations › Conference presentations

**PhD defense (opponent): Manuel Placencia Gutierrez, "Searching for saddle points and global minima***
Period: 20 Oct 2015
Tejs Vegge (External examiner)
Center for Atomic-scale Materials Design
BACHU NARAIN SINGH: ENDURING IMPACT ON RADIATION DAMAGE PHYSICS
Morten Mostgaard Eldrup (Speaker)

Description
Talk given by 1st author of abstract at '17th International Conference on Fusion Reactor Materials'

Participate as author

Co-authors: S.J. Zinkle1,2, M. Eldrup3, S.A. Fabritsiev4, N.M. Ghoniem5, S.I. Golubov2, H.L. Heinisch6, S. Ishino7, Yu.N. Osetsky2, and M. Victoria81University of Tennessee, Knoxville, TN 37996, USA2Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA3Technical University of Denmark, Risø Campus, Roskilde, Denmark4D.V. Efremov Scientific Research Inst., St. Petersburg, Russia5University of California, Los Angeles, CA, USA6Pacific Northwest National Laboratory, Richland, WA, USA7University of Tokyo, Hongo, Bunkyo-ku, Tokyo 113-8654, Japan8CRPP, Villigen, Switzerland

Related event
17th International Conference on Fusion Reactor Materials
11/10/2015 → 16/10/2015
Aachen, Germany
Activity: Talks and presentations › Conference presentations

Ionic and electronic transport properties in LiFeBO3 from DFT
Tejs Vegge (Invited speaker)

Description
Workshop on understanding interfaces in electrochemical storage systems

Related event
Workshop on Understanding Interfaces in Electrochemical Storage Systems
06/10/2015 → 08/10/2015
Tours, France
Activity: Talks and presentations › Conference presentations
Tours, France
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

The 66th Annual Meeting of the International Society of Electrochemistry
Anne Hauch (Participant)
Department of Energy Conversion and Storage
Applied Electrochemistry

Description
International Society of Electrochemistry 66th annual meeting

Related event
The 66th Annual Meeting of the International Society of Electrochemistry
04/10/2015 → 09/10/2015
Taipei, Taiwan, Province of China
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

ELECTROCHEMICAL CONVERSION OF CO2 INTO LIQUID FUEL ON RuO2 (110) OVERLAYERS
Period: 2 Oct 2015
Arghya Bhowmik (Lecturer)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related event
Annual Meeting of the Danish Electrochemical Society 2015
01/10/2015 → 02/10/2015
Copenhagen, Denmark
Activity: Talks and presentations › Conference presentations

Annual Meeting of the Danish Electrochemical Society 2015
Period: 1 Oct 2015 → 2 Oct 2015
Mateusz Krzysztof Reda (Speaker)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Description
Poster presentation

Annual Meeting of the Danish Electrochemical Society 2015

Related event
Annual Meeting of the Danish Electrochemical Society 2015
01/10/2015 → 02/10/2015
Copenhagen, Denmark
Activity: Talks and presentations › Conference presentations

ISOS-8
Period: 1 Oct 2015
Michael Corazza (Speaker)
Department of Energy Conversion and Storage
Functional organic materials

**Description**
ISOS-8

**Links:**

**Related event**
ISOS-8
29/09/2015 → 01/10/2015
Rio de Janeiro, Brazil
Activity: Talks and presentations › Conference presentations

**PhD defense (opponent):** Kristian Baruel Ørnsø, "Computational design of molecules for dye sensitized solar cells and nano electronics"
Period: 1 Oct 2015
Tejs Vegge (Internal examiner)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Activity: Examinations and supervision › Internal examination

**Nye Energiteknologier: Danmarks fremtidige energisystem uden fossile brændstoffer – Brændselsceller og elektrolyse**
Period: Sep 2015 → Oct 2015
Anke Hagen (Participant)
Department of Energy Conversion and Storage
Applied Electrochemistry

**Related external organisation**
DTU Energy
Roskilde, Denmark
Activity: Other

**Polybenzimidazole membranes in alkaline water electrolysis: Chemical and electrochemical stability**
Period: 29 Sep 2015 → 1 Oct 2015
Mikkel Rykær Kraglund (Other)
Department of Energy Conversion and Storage
Proton conductors
Degree of recognition: International
Documents:
3DegIs poster v2

**Related event**
International workshop on degradation issues of fuel cells and electrolyzers
29/09/2015 → 01/10/2015
Thira, Greece
Activity: Talks and presentations › Conference presentations

**Electricity Storage in Batteries**
Period: 28 Sep 2015
Related event

Energy storage – a must for successful conversion to green energy
28/09/2015 → …
Danish Academy of Technical Sciences (ATV), Denmark
Activity: Talks and presentations › Conference presentations

Energy Supply Modelling in Cities: Illustrated Using Data from the Danish Municipality of Sønderborg
Period: 28 Sep 2015
Dadi Þorsteinn Sveinbjörnsson (Keynote speaker)
Department of Energy Conversion and Storage
Description
Session keynote presentation
Related event

10th Conference on Sustainable Development of Energy, Water and Environment Systems
27/09/2015 → 02/10/2015
Dubrovnik, Croatia
Activity: Talks and presentations › Conference presentations

Er der vedvarende energi nok til os alle?
Period: 21 Sep 2015 → 25 Sep 2015
Anne Hauch (Lecturer)
Department of Energy Conversion and Storage
Related event

Dansk Naturvidenskabsfestival 2015
21/09/2015 → 25/09/2015
Denmark
Activity: Talks and presentations › Conference presentations

4th Metal-air Workshop
Period: 14 Sep 2015 → 15 Sep 2015
Rune Christensen (Speaker)
Atomic scale modelling and materials
Department of Energy Conversion and Storage
Center for Atomic-scale Materials Design
Description
Reducing Systematic Errors in OxideSpecies with DensityFunctional Theory Calculations
ReLiable Metal-air battery workshop
Related event

4th Metal-air Workshop: The Road Ahead
14/09/2015 → 15/09/2015
Copenhagen, Denmark
IN SITU SMALL ANGLE STUDIES OF ROLL-TO-ROLL COATED PEROVSKITE SOLAR CELLS
Period: 14 Sep 2015
Lea Hildebrandt Rossander (Speaker)
Department of Energy Conversion and Storage
Organic Energy Materials

Related event
16th Conference on Small Angle Scattering (SAS 2015)
13/09/2015 → 18/09/2015
Berlin, Germany
Activity: Talks and presentations › Conference presentations

In situ GISAXS/GIWAXS studies of roll-to-roll coated perovskite solar cells
Period: 10 Sep 2015
Lea Hildebrandt Rossander (Speaker)
Department of Energy Conversion and Storage
Organic Energy Materials

Related event
GISAS2015: 3rd International GISAS Conference
08/09/2015 → …
Nice, France
Activity: Talks and presentations › Conference presentations

PSI-K 2015 Conference
Period: 6 Sep 2015 → 10 Sep 2015
Simon Loftager (Participant)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Description
Poster presentations: "Computational investigations of transport mechanisms across battery interfaces" and "How should the energies of localized vs. delocalized polarons be compared in supercell calculations? A case study in self-trapped polarons in silver halides"

Psi-k 2015 conference

Related event

PSI-K 2015 Conference
06/09/2015 → 10/09/2015
San Sebastian, Spain
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Energy Supply Modelling in Cities: Illustrated Using Data from the Case of Sønderborg
Period: 1 Sep 2015
Dadi Þorsteinn Sveinbjörnsson (Speaker)
Department of Energy Conversion and Storage

Related event
Nordic Climate KIC - CITIES workshop
01/09/2015 → …
Copenhagen, Denmark
Activity: Talks and presentations › Conference presentations

Journal of Fuel Cell Science and Technology (Journal)
Period: 1 Sep 2015 → 31 Aug 2018
Jacob R. Bowen (Editor)
Department of Energy Conversion and Storage
Imaging and Structural Analysis

Description
Journal of Fuel Cell Science and Technology

Associate Editor

Links:
http://fuelcellscience.asmedigitalcollection.asme.org (Journal of Fuel Cell Science and Technology homepage)
http://journaltool.asme.org/Content/Masthead19.cfm (Editorial Board)

Related journal
Journal of Fuel Cell Science and Technology
1550-624X
Central database
Activity: Research › Journal editor

Novel Heterostructured and Multilayered Oxide Thin Films for Future Applications
Period: 1 Sep 2015 → 4 Sep 2015
Søren Linderoth (Keynote speaker)
Department of Energy Conversion and Storage

Related event
Donostia International Workshop on Energy Materials Nanotechnology
01/09/2015 → 04/09/2015
San Sebastian - Donostia (Guipuzcoa), Spain
Activity: Talks and presentations › Conference presentations

University of the Basque Country
Period: 1 Sep 2015 → 30 Sep 2015
Simon Loftager (Visiting researcher)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Description
External research stay at Nano-bio Spectroscopy Group, University of the Basque Country
Activity: Visiting an external institution › Visiting another research institution

Journal of Electrochemical Energy Conversion and Storage (Journal)
Period: 31 Aug 2015 → 31 Aug 2018
Jacob R. Bowen (Editor)
Department of Energy Conversion and Storage
Imaging and Structural Analysis
Degree of recognition: International
Links:
https://journaltool.asme.org/home/Mastheads.cfm?JournalID=30 (Masthead)

Related journal
Journal of Electrochemical Energy Conversion and Storage
2381-6872
Scopus rating (2017): CiteScore 1.27 SJR 0.308 SNIP 0.301, Web of Science (2018): Indexed yes
Local database
Activity: Research › Journal editor

Ionic and electronic transport in solid oxide cells – Seen from an applied perspective
Period: 25 Aug 2015
Anke Hagen (Invited speaker)
Department of Energy Conversion and Storage
Applied Electrochemistry

Related event
15th European Conference on Solid State Chemistry
23/08/2015 → 26/08/2015
Vienna, Austria
Activity: Talks and presentations › Conference presentations

European School of Magnetism
Period: 24 Aug 2015 → 4 Sep 2015
Andrea Roberto Insinga (Participant)
Department of Energy Conversion and Storage
Electrofunctional materials

Description
From fundamental magnetism to spin currents

Related event
European School of Magnetism
24/08/2015 → 04/09/2015
Cluj-Napoca, Romania
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Materials for Energy Storage – and how DFT can improve them
Tejs Vegge (Invited speaker)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related event
SUNCAT Summer Institute 2015
24/08/2015 → 28/08/2015
Stanford, United States
Activity: Talks and presentations › Conference presentations
SUNCAT Summer Institute 2015
Rune Christensen (Participant)
Department of Energy Conversion and Storage
Atomic scale modelling and materials
Description
Poster presentation given
Summer workshop on catalysis at Stanford

Related event
SUNCAT Summer Institute 2015
24/08/2015 → 28/08/2015
Stanford, United States
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

SUNCAT Summer Institute 2015
Simon Loftager (Participant)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials
Description
Poster presentation: “Computational investigations of transport mechanisms across battery interfaces”
Suncat Summer Institute 2015, SLAC National Accelerator Laboratory & Stanford University

Related event
SUNCAT Summer Institute 2015
24/08/2015 → 28/08/2015
Stanford, United States
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

SUNCAT Summer Institute 2015
Mateusz Krzysztof Reda (Participant)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials
Description
Poster presentation
SUNCAT Summer Institute (summer school)

Related event
SUNCAT Summer Institute 2015
24/08/2015 → 28/08/2015
Stanford, United States
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Improved Accuracy of Density Functional Theory Calculations for CO2 Reduction and Metal-Air Batteries
Period: 19 Aug 2015
Rune Christensen (Lecturer)
Atomic scale modelling and materials
Department of Energy Conversion and Storage

**Description**
Lecture given while visiting Catalyst Design Lab at Brown University
Lecture about my work given to the Catalyst Design Lab at Brown University

**Related external organisation**
**Unknown external organisation**
Activity: Talks and presentations › Conference presentations

**Brown University**
Rune Christensen (Visiting researcher)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

**Description**
External stay at Catalyst Design Lab
Activity: Visiting an external institution › Visiting another research institution

**Brown University**
Rune Christensen (Visiting researcher)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

**Description**
Visit at Brown University: Catalyst Design Lab
Activity: Visiting an external institution › Visiting another research institution

**The Danish SOC Landscape 2015**
Period: 1 Aug 2015
Anke Hagen (Invited speaker)
Department of Energy Conversion and Storage
Applied Electrochemistry

**Related event**
**IEA Annex SOFC**
01/08/2015 → 01/08/2015
Glasgow, United Kingdom
Activity: Talks and presentations › Conference presentations

**On the Challenge of Stabilizing Contacts in Bi-Te Thermoelectric Generator under thermal cycling**
Period: 24 Jun 2015 → 26 Jun 2015
Ngo Van Nong (Invited speaker)
Department of Energy Conversion and Storage
Electrofunctional materials

**Related event**
**Energy Harvesting Systems - FlexTEG 2015**
Atomic-scale modeling of materials for hydrogen-based energy storage
Period: 22 Jun 2015 → 26 Jun 2015
Tejs Vegge (Invited speaker)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related event
4th European Technical School on Hydrogen and Fuel Cells
22/06/2015 → 26/06/2015
Crete, Greece
Activity: Talks and presentations › Conference presentations

Towards a Fossil-Free Energy System: How Possible to Achieve?
Period: 29 May 2015
Søren Linderoth (Invited speaker)
Department of Energy Conversion and Storage
Description
Clean Energy Forum: "Towards a Fossil-Free Energy System: How Possible to Achieve?"

Related event
Clean Energy Forum
29/05/2015 → …
Beijing, China
Activity: Talks and presentations › Conference presentations

Rare earth-transitional metal oxides and compounds for environment-friendly energy science and technology
Period: 26 May 2015
Søren Linderoth (Invited speaker)
Department of Energy Conversion and Storage
Description
Introduction to DTU Energy

Related event
Rare earth-transitional metal oxides and compounds for environment-friendly energy science and technology
26/05/2015 → 27/05/2015
Beijing, China
Activity: Talks and presentations › Conference presentations

Rare earth-transitional metal oxides and compounds for environment-friendly energy science and technology
Period: 26 May 2015
Christian Bahl (Invited speaker)
Department of Energy Conversion and Storage
Electrofunctional materials

Related event
Rare earth-transitional metal oxides and compounds for environment-friendly energy science and technology
26/05/2015 → 27/05/2015
Beijing, China
Status and Results of Energy Supply Modelling in CITIES: Illustrated using Data from the Case of Sønderborg
Period: 26 May 2015
Dadi Þorsteinn Sveinbjörnsson (Lecturer)
Department of Energy Conversion and Storage
Centre for IT-Intelligent Energy Systems in Cities

Related event
CITIES Second General Consortium Meeting
26/05/2015 → 27/05/2015
Kgs. Lyngby, Denmark

Activity: Talks and presentations › Conference presentations

227th ECS Meeting
Rune Christensen (Speaker)
Atomic scale modelling and materials
Department of Energy Conversion and Storage

Description
Improved Accuracy of Density Functional Theory Calculations for CO2 Reduction and Metal-Air Batteries

Speaking at and participating in 227th ECS Meeting

Related event
227th ECS Meeting
24/05/2015 → 28/05/2015
Chicago, IL, United States

Activity: Talks and presentations › Conference presentations

Vedvarende energi: Ny teknologi, der ændrer vores hverdag
Period: 20 May 2015
Anne Hauch (Lecturer)
Department of Energy Conversion and Storage
Applied Electrochemistry

Description
Foredrag om vedvarende energi og energikonvertering og lagring i forelæsningsserie om "Ny teknologi" på Aarhus Folkeuniversitet (Emdrup afd.)

Related external organisation
Unknown external organisation

Activity: Talks and presentations › Conference presentations

PhD defense (member of evaluation committee): Edith Ahlberg Helgee, "Significance of grain boundaries for transport phenomena in graphene and proton-conducting barium zirconate" at Chalmers University of Technology, Sweden
(External organisation)
Period: 8 May 2015
Tejs Vegge (External examiner)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials
Brændselceller og elektrolyse: En del af løsningen for fremtidens energiudfordringer
Period: Apr 2015
Anke Hagen (Invited speaker)
Department of Energy Conversion and Storage
Applied Electrochemistry
Description
Public presentation: Bestil en Forsker

Related event

Bestil en forsker: Forskningens Døgn
22/04/2015 → 26/04/2015
Sønderborg, Denmark
Activity: Talks and presentations › Conference presentations

Forskningens Døgn 2015
Period: Apr 2015
Anke Hagen (Participant)
Department of Energy Conversion and Storage
Applied Electrochemistry
Description
Forskningens Døgn: Exhibition Roskilde

Related event

Forskningens Døgn 2015
22/04/2015 → 26/04/2015
Denmark
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Workshop on Advancing Caloric Materials for Efficient Cooling
Period: 29 Apr 2015
Christian Bahl (Invited speaker)
Department of Energy Conversion and Storage
Electrofunctional materials
Description
Workshop on Advancing Caloric Materials for Efficient Cooling

Related event

Workshop on Advancing Caloric Materials for Efficient Cooling
28/04/2015 → 29/04/2015
College Park, Maryland, United States
Activity: Talks and presentations › Conference presentations

Novel electrodes for efficient and durable electrolysis and fuel cells
Period: 28 Apr 2015 → 29 Apr 2015
Peter Holtappels (Invited speaker)
Department of Energy Conversion and Storage
Fundamental Electrochemistry
Description
Novel electrodes for efficient and durable electrolysis and fuel cells

Related event

**EERA Inter-JP cross-fertilization workshop on materials for energy applications and technologies**
Period: 28/04/2015 → 29/04/2015
Brussels, Denmark
Activity: Talks and presentations › Conference presentations

### 3rd Conference on Frontiers of Aberration Corrected Electron Microscopy
**Period:** 19 Apr 2015 → 23 Apr 2015
**Location:** Kasteel Vaalsbroek, Netherlands
**Activity:** Talks and presentations › Conference presentations

**Description**
Poster presentation at PICO conference 2015
Degree of recognition: International
Documents:
Abstract

**Related event**

3rd Conference on Frontiers of Aberration Corrected Electron Microscopy
19/04/2015 → 23/04/2015
Kasteel Vaalsbroek, Netherlands
Activity: Talks and presentations › Conference presentations

**Manufacturing of Green Fuels from Renewable Energy**
**Period:** 16 Apr 2015
**Location:** Lyngby, Denmark
**Activity:** Talks and presentations › Conference presentations

**Description**
Poster presentation on "The Influence of Electronic Structure on H/OH/CO Binding Energy on Rutile (110) Oxide Surfaces"

**Related event**

Manufacturing of Green Fuels from Renewable Energy
14/04/2015 → 16/04/2015
Lyngby, Denmark
Activity: Talks and presentations › Conference presentations

**High Temperature Alkaline Electrolysis - Progress and Potential**
**Period:** 15 Apr 2015
**Location:** Lyngby, Denmark
**Activity:** Talks and presentations › Conference presentations

**Related event**

Manufacturing of Green Fuels from Renewable Energy
14/04/2015 → 16/04/2015
Lyngby, Denmark
Activity: Talks and presentations › Conference presentations
Integration of improved correction schemes and operational conditions in the design of nanoalloy catalysts for CO2 reduction
Period: 14 Apr 2015 → 16 Apr 2015
Tejs Vegge (Invited speaker)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related event

Manufacturing of Green Fuels from Renewable Energy
Period: 14 Apr 2015 → 16 Apr 2015
Lyngby, Denmark
Activity: Talks and presentations › Conference presentations

Manufacturing of Green Fuels from Renewable Energy
Period: 14 Apr 2015 → 16 Apr 2015
Rune Christensen (Speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Description
Participant and poster presenter
Workshop on Manufacturing of Green Fuels from Renewable Energy

Related event

Manufacturing of Green Fuels from Renewable Energy
Period: 14 Apr 2015 → 16 Apr 2015
Lyngby, Denmark
Activity: Talks and presentations › Conference presentations

MRS Spring Meeting
Period: 6 Apr 2015 → 10 Apr 2015
Qingfeng Li (Invited speaker)
Department of Energy Conversion and Storage
Proton conductors

Description
Iron carbide nanoparticles encapsulated by graphitic layers as ORR catalysts. Abstract on NPMC
Invited talk
Documents:
Abstract on NPMC - MRS Spring Meeting, 6- 10 April 2015, San Francisco, California

Related event

2015 MRS Spring Meeting & Exhibit
06/04/2015 → 10/04/2015
San Francisco, United States
Activity: Talks and presentations › Conference presentations

Design of borohydrides and novel materials for ammonia storage
Period: 18 Mar 2015
Tejs Vegge (Invited speaker)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related event
IEA-teknologinetværk om brint og brændselsceller og FCH2-programmet
18/03/2015 → 
Copenhagen, Denmark
Activity: Talks and presentations › Conference presentations

American Physical Society March Meeting 2015
Period: 3 Mar 2015
Kurt Engelbrecht (Participant)
Department of Energy Conversion and Storage
Electrofunctional materials

Description
Presented Invited talk titled: "Modelling and Design Aspects of Active Caloric Regenerators"

American Physical Society March Meeting
Links:
http://www.aps.org/meetings/march/index.cfm

Related event
American Physical Society March Meeting 2015
02/03/2015 → 06/03/2015
San Antonio, United States
Activity: Attending an event › Participating in or organising a conference

Asilomar 2015
Period: 10 Feb 2015
Qingfeng Li (Invited speaker)
Department of Energy Conversion and Storage
Proton conductors

Description
High Temperature Durable Membranes for Fuel Cells

Invited talk
Degree of recognition: International
Documents:
Abstract submitted to Advances in Polymers for Fuel Cells and Energy Devices Qingfeng Li

Related event
Asilomar 2015: Advances in Polymers for Fuel Cells and Energy Devices
08/02/2015 → 11/02/2015
Pacific Grove, United States
Activity: Talks and presentations › Conference presentations

Energiforvandling - Brændselsceller og brint: Vedvarende Energi
Period: 10 Feb 2015
Anne Hauch (Lecturer)
Department of Energy Conversion and Storage
Applied Electrochemistry

**Description**
Forelæsning om brændselceller og bring i forelæsningsserien "Vedvarende Energi" på Aarhus Folkeuniversitet (Emdrup afdeling)

**Related external organisation**

**Unknown external organisation**
Activity: Talks and presentations › Conference presentations

**SUNCAT Center for Interface Science and Catalysis**
Period: 8 Feb 2015 → 1 Mar 2015
Rune Christensen (Visiting researcher)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

**Description**
External stay at SUNCAT
Stay at SUNCAT center at Stanford
Activity: Visiting an external institution › Visiting another research institution

**Material & Struktur – Entscheidende Kombination für Hochtemperaturbrennstoff- und Elektrolysezellen**
Period: 27 Jan 2015
Anke Hagen (Invited speaker)
Department of Energy Conversion and Storage
Applied Electrochemistry

**Related event**

**Karlsruher Werkstoffkolloquium**
27/01/2015 → ...
Karlsruhe, Germany
Activity: Talks and presentations › Conference presentations

**39th International Conference and Expo on Advanced Ceramics and Composites**
Period: 25 Jan 2015 → 30 Jan 2015
Vincenzo Esposito (Organizer)
Department of Energy Conversion and Storage
Ceramic Engineering & Science

**Description**
11th International Symposium on Solid Oxide Fuel Cells (SOFC): Materials, Science and Technology
Links:

**Related event**

**39th International Conference and Expo on Advanced Ceramics and Composites**
25/01/2015 → 30/01/2015
Daytona Beach, FL, United States
Activity: Attending an event › Participating in or organising a conference

**Materials Predictors and Genetic Algorithms for Rational Design of Electrocatalytic Nanoparticles**
Period: 7 Jan 2015 → 11 Jan 2015
Tejs Vegge (Invited speaker)
9th International Conference on Computational Physics
07/01/2015 → 11/01/2015
Singapore, Singapore
Activity: Talks and presentations › Conference presentations

6th IIR/IIF International Conference on Magnetic Refrigeration
Period: 2014
Henrique Neves Bez (Participant)
Department of Energy Conversion and Storage
Electrofunctional materials

Description
Poster presentation on thermal hysteresis of manganite

Angewandte Chemie (International Edition) (Journal)
Period: 2014
Tejs Vegge (Reviewer)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related journal
Angewandte Chemie International Edition
1433-7851
Web of Science (2018): Indexed yes
Central database
Activity: Research › Peer review of manuscripts

Applied Catalysis A-general (Journal)
Period: 2014
Anke Hagen (Reviewer)
Department of Energy Conversion and Storage
Applied Electrochemistry

Related journal
Applied Catalysis A-general
0926-860X
Web of Science (2018): Indexed yes
Central database
Activity: Research › Peer review of manuscripts
Årsmøde 2014 i Dansk Batteriselskab
Period: 2014 → …
Jonathan Højberg (Organizer)
Department of Energy Conversion and Storage
Atomic scale modelling and materials
Links:
http://batteriselskab.dk/danish-battery-symposium-2014

Related event

Årsmøde 2014 i Dansk Batteriselskab
28/02/2014 → …
Lyngby, Denmark
Activity: Attending an event › Participating in or organising a conference

Chemical Review (Journal)
Period: 2014
Tejs Vegge (Reviewer)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related journal

Chemical Review
Local database
Activity: Research › Peer review of manuscripts

Fuel Cells (Journal)
Period: 2014
Tejs Vegge (Reviewer)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related journal

Fuel Cells
1615-6846
BFI (2018): BFI-level 1, Scopus rating (2017): CiteScore 1.88 SJR 0.559 SNIP 0.748, ISI indexed (2013): ISI indexed yes, Web of Science (2018): Indexed yes
Central database
Activity: Research › Peer review of manuscripts

HyFC Academy PhD Workshop on Catalysts for Fuel Cells and Electrolysers
Period: 2014
James Atwoki Mugabi (Participant)
Department of Energy Conversion and Storage
Proton conductors

Description
HyFC (The Danish Hydrogen and Fuel cell academy, 2014)

Related event
HyFC Academy PhD Workshop on Catalysts for Fuel Cells and Electrolysers
13/02/2014 → …
Lyngby, Denmark
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Journal of Chemical Physics (Journal)
Period: 2014
Tejs Vegge (Reviewer)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related journal
Journal of Chemical Physics
0021-9606
BFI (2018): BFI-level 2, Scopus rating (2017): CiteScore 2.5 SJR 1.252 SNIP 0.926, ISI indexed (2013): ISI indexed yes,
Web of Science (2018): Indexed yes
Central database
Activity: Research › Peer review of manuscripts

Nature Chemistry (Journal)
Period: 2014
Tejs Vegge (Reviewer)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related journal
Nature Chemistry
1755-4330
Web of Science (2018): Indexed yes
Central database
Activity: Research › Peer review of manuscripts

Nature Materials (Journal)
Period: 2014
Tejs Vegge (Reviewer)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related journal
Nature Materials
1476-1122
Web of Science (2018): Indexed yes
Central database
Activity: Research › Peer review of manuscripts

Optical antennas, optical cavity and photonic crystals to enhance the performance of organic solar cells
Period: 2014
Francesco Pastorelli (Speaker)
Department of Energy Conversion and Storage

Functional organic materials

**Related event**

**E-MRS 2014 Spring Meeting**
25/05/2014 → 30/05/2014
Lille, France
Activity: Talks and presentations › Conference presentations

**QuantumHagen**
Period: 2014 → …
Rune Christensen (Participant)
Department of Energy Conversion and Storage

**Related event**

**QuantumHagen: Workshop on Modeling of Electronic Devices and Materials at the Nanoscale**
01/07/2014 → 03/07/2014
Copenhagen, Denmark
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

**Referee for Netherlands Organisation for Scientific Research (NWO) - Chemical Sciences (External organisation)**
Period: 2014
Tejs Vegge (Member)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials
Degree of recognition: International

**Related external organisation**

**Referee for Netherlands Organisation for Scientific Research (NWO) - Chemical Sciences**
Activity: Membership › Membership in review committee

**Referee for US Department of Energy (DoE), Energy Frontiers Research Centers (EFRC) (External organisation)**
Period: 2014
Tejs Vegge (Member)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials
Degree of recognition: International

**Related external organisation**

**Referee for US Department of Energy (DoE), Energy Frontiers Research Centers (EFRC)**
Activity: Membership › Membership in review committee

**ReLiable Workshop III**
Period: 2014
Rune Christensen (Participant)
Atomic scale modelling and materials
Department of Energy Conversion and Storage

**Related event**
Semitransparent Organic Solar Cell toward Opaque Performances
Period: 2014 → …
Francesco Pastorelli (Speaker)
Department of Energy Conversion and Storage
Functional organic materials

Related event

2014 MRS Spring Meeting
21/04/2014 → 25/04/2014
San Francisco, United States
Activity: Talks and presentations › Conference presentations

The Journal of Physical Chemistry Part C: Nanomaterials, Interfaces and Hard Matter (Journal)
Period: 2014
Tejs Vegge (Reviewer)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related journal

The Journal of Physical Chemistry Part C
1932-7447
BFI (2018): BFI-level 1, Scopus rating (2017): CiteScore 4.58 SJR 2.135 SNIP 1.147, ISI indexed (2013): ISI indexed yes,
Web of Science (2018): Indexed yes
Central database
Activity: Research › Peer review of manuscripts

Elchemea Data Acquisition: Software til impedansspektroskopi, cyklisk voltametri samt chronopotentiometri/amperometri
Period: Dec 2014
Søren Koch (Participant)
Department of Energy Conversion and Storage
Applied Electrochemistry

Description
Open source software pakke til opsamling af impedans spektr, cyklisk voltametri og chrono-potentiometri/amperometri
offentliggjort under GPL

Head : Søren Kock
Links:
http://www.elchemea.com/elchemea/
Activity: Other

Scalable Roll-to-Roll Fabrication for Fully Solution-Processed Polymer Solar Cells from Small-Scale Test Devices to Multi Square Meter Large Modules for Energy Production
Period: 3 Dec 2014
Markus Hösel (Speaker)
Department of Energy Conversion and Storage
Functional organic materials
The majority of lab-scale organic and polymer solar cells (OPV) are very small with <<0.5 cm² using ITO glass, spin coating, evaporation, inert atmosphere, and optimum conditions. Obviously, the cells can lead to record efficiencies - but they are far beyond real world applications due to miniscule power output. Transfer to large-scale devices with an appropriate power output is hardly possible.

Here, we present the route from roll and roll-to-roll processed test devices to multi square meter large polymer solar cell modules with hundreds of Watts output - fully roll-to-roll (R2R) produced under vacuum-free and ambient conditions without using indium tin oxide (ITO) as transparent conductive electrode. ITO has the highest impact on the embodied energy in OPV devices and is replaced by an all additive printed and coated electrode based on flexo printed silver grid, rotary screen printed PEDOT:PSS, and slot-die coated zinc oxide (Flextrode). The production speed for each layer is beyond 10 m/min independently of the individual layout for different devices.

Model cells with at least 1 cm² are fabricated on a rollcoater, which allows easy transfer to the R2R line for larger test modules with e.g. 8 serially connected cells and the size of a postcard (freeOPV, active area >50 cm²). Both routes allow the testing of new polymers, functional inks, and device structures such as tandem stacks with minimum amount of material input but large number of devices for statistical analyses.

Finally, OPV modules with high power output for real-world applications and grid-connection can be easily produced based on the Infinity concept developed in our group. Virtually infinite large solar cell modules are based on thousands of serially connected cells entirely fabricated using very fast R2R printing and coating processes. No manual labour or proprietary processes are required for bussing and interconnection of submodules. The serial connection is completed throughout the print run due to an optimized pattern layout. The advantage of the Infinity concept is the fabrication of high-voltage OPV modules with active areas beyond several square meters (21000 cells = 14.7 m², 100 m long) and stabilized power outputs of >220 W using the standard active layer material P3HT:PCBM. The module has only two terminal connectors for minimized wiring during the setup of module arrays. The installation of a 100 m long module takes less than one minute. A parallel-connected array with outputs >1.3 kW and rather low efficient material (<2%) was built. An entire solarpark based on such OPV modules has a low energy payback time of just 0.5 years.

Related event
2014 MRS Fall Meeting & Exhibit
30/11/2014 → 05/12/2014
Boston, United States
Activity: Talks and presentations › Conference presentations

International Carisma Conference
Period: 1 Dec 2014 → 3 Dec 2014
Jens Oluf Jensen (Speaker)
Department of Energy Conversion and Storage
Proton conductors

Description

Related event
International Carisma Conference
01/12/2014 → 03/12/2014
Cape Town, South Africa
Activity: Talks and presentations › Conference presentations

2014 MRS Fall Meeting & Exhibit
Period: 30 Nov 2014 → 5 Dec 2014
Simona Ovtar (Participant)
Department of Energy Conversion and Storage
Mixed Conductors

Description
Enhanced oxygen exchange of (La₀.₆Sr₀.₄)₀.₉₉FeO₃₋₋₅ – Ce₀.₉Gd₀.₁O₁.₉₅ composites
Documents:
abstract

Related event
Conference on Energy and Environment for the Future
Emil Bøje Lind Pedersen (Speaker)
Imaging and Structural Analysis
Department of Energy Conversion and Storage
Description
Presented a poster titled: "Ptychographic Tomography of an organic tandem solar cell".

Participated in "Energy and Environment for the future".

Related event
Conference on Energy and Environment for the Future: Sustainable energy for a fossil free society and environmentally friendly technologies
Copenhagen, Denmark
Activity: Talks and presentations › Conference presentations

Conference on Energy and Environment for the Future
Jens Oluf Jensen (Speaker)
Department of Energy Conversion and Storage
Proton conductors
Description

Related event
Conference on Energy and Environment for the Future: Sustainable energy for a fossil free society and environmentally friendly technologies
Copenhagen, Denmark
Activity: Talks and presentations › Conference presentations

Børnenes Universitet 2014
Period: 22 Nov 2014
Anke Hagen (Organizer)
Department of Energy Conversion and Storage
Applied Electrochemistry
Description
Børnenes Universitet: Workshop Vi fanger Solen

Related event
Børnenes Universitet 2014
22/11/2014 → …
Kgs. Lyngby, Denmark
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.
Andet symposium hos Institut for Energikonvertering- og lagring
Period: 21 Nov 2014
Simon Loftager (Participant)
Center for Atomic-scale Materials Design
Department of Physics
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related event

Andet symposium hos Institut for Energikonvertering- og lagring
21/11/2014 → …
Kgs. Lyngby, Denmark
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Positron Annihilation Spectroscopy on LiBH4 and LiBH4:LiI superionic lithium conductors
Period: 13 Nov 2014
Morten Mostgaard Eldrup (Lecturer)
Department of Energy Conversion and Storage
Atomic scale modelling and materials
Documents:
Eldrup_PPC11-abstractX
Eldrup_PPC11_abstractX.pdf
Links:
http://www.barc.gov.in/symposium/ppc11/

Related event

11th International Workshop on Positron and Positronium Chemistry
09/11/2014 → 14/11/2014
Goa, India
Activity: Talks and presentations › Conference presentations

Overpotentials and Transport Mechanisms in Metal-air Batteries
Period: 12 Nov 2014
Tejs Vegge (Invited speaker)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related event

EEWS Workshop: Advanced Technology for Next Generation Energy Storage System
12/11/2014 → …
Daejeon, Korea, Republic of
Activity: Talks and presentations › Conference presentations

Symposium on Nanoscale Thermal Transport
Period: 10 Nov 2014
Kaspar Kirstein Nielsen (Participant)
Department of Energy Conversion and Storage
Electrofunctional materials
Description
Nanothermal transport

Related event

Symposium on Nanoscale Thermal Transport
10/11/2014 → 10/11/2014
Gothenburg, Sweden
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

High temperature electrolysis activities at Technical University of Denmark
Period: 7 Nov 2014
Sune Dalgaard Ebbesen (Invited speaker)
Department of Energy Conversion and Storage
Applied Electrochemistry
Documents:
leafletfuelcells-3

Related event

Fuel Cells & Electrolysers Energy for the future
07/11/2014 → …
Barcelona, Spain
Activity: Talks and presentations › Conference presentations

The Needs for Storage/Flexibility in the Danish Energy System: Drivers, application areas and requirements
Period: 5 Nov 2014
Allan Schrøder Pedersen (Lecturer)
Department of Energy Conversion and Storage
Description
An overview of expected need for energy storage in the future Danish energy system was given in collaboration with Energinet.dk. In addition recommended storage technologies relevant in a Danish context were pointed out.

Presentation given in collaboration with Energinet.dk

Related event

European Utility Week
04/11/2014 → 06/11/2014
Amsterdam, Netherlands
Activity: Talks and presentations › Conference presentations

Metal-air Batteries: Fundamental Mechanisms and Limitations
Period: 4 Nov 2014 → 6 Nov 2014
Tejs Vegge (Invited speaker)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related event

Materials for Tomorrow
04/11/2014 → 06/11/2014
Gothenburg, Sweden
Activity: Talks and presentations › Conference presentations
Optimization model for transportation fuels and SNG production from renewable sources in Denmark: Master Thesis
Alessia Elia
Period: 1 Nov 2014 → 1 Jul 2015
Allan Schrøder Pedersen (Supervisor)
Centre for IT-Intelligent Energy Systems in Cities
Department of Energy Conversion and Storage

Description
The purpose of this Master Thesis was to create an optimization tool for the analysis of fuels production for transportation and SNG1 for residential and industrial sectors using renewable energy. The system analyzed is mainly focused on the possible paths to obtain fuels using biomass and hydrogen (produced using electrolysis) as input and all the connections to combine these resources and energy vector in the best way. After a brief introduction and theoretical presentation, in chapter 3 the system analyzed is explained and the model is developed. In Chapter 4 the data and values adopted in the model are presented. The model is designed to minimize the breakeven cost of the system satisfying the energy demand. Finally, a wide category of scenarios were run, each distinguished by different choices of energy demand or technology processes. In the end, some of these scenarios were performed in sensitivity analyses regarding the amount of energy resources, their price, and the obligations of production using certain pathways. The model gives the possibility to investigate different parameters but results obtained were mainly focused about the amount of energy inputs consumed and the break-even cost. For each analysis the solver computes a meaningful solution which suggests different combination of energy inputs and technology to use.

Magnetic Materials and Applications seminar
Christian Bahl (Participant)
Department of Energy Conversion and Storage
Electrofunctional materials

Related event
Magnetic Materials and Applications seminar
28/10/2014 → 29/10/2014
Lucerne, Switzerland
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

International Conference on X-Ray Microscopy
Emil Bøje Lind Pedersen (Speaker)
Imaging and Structural Analysis
Department of Energy Conversion and Storage

Description
Presented a poster titled: “Ptychographic Tomography of an Organic Tandem Solar Cell Containing Active Layers Cast from Solution and Water-Dispersable Nano Particles”
Poster presentation at XRM (International X-Ray Microscopy Conference 2014)

Related event
International Conference on X-Ray Microscopy
26/10/2014 → 31/10/2014
Melbourne, Australia
Activity: Talks and presentations › Conference presentations

Solid oxide cells: Smart electrochemical devices for the smart energy systems of the future
Period: 22 Oct 2014
Anke Hagen (Invited speaker)
Department of Energy Conversion and Storage

Period: 14 Oct 2014
Vincenzo Esposito (Invited speaker)
Department of Energy Conversion and Storage
Ceramic Engineering & Science

Description
Materials Science & Technology 2014
Links:

The Focused Ion Beam – Scanning Electron Microscope: A tool for sample preparation, two and three dimensional imaging

Period: 13 Oct 2014
Jacob R. Bowen (Guest lecturer)
Department of Energy Conversion and Storage
Imaging and Structural Analysis

Description
Remote teaching guest lecture (2 hours) as part of The Univerity of Connecticut course: ME3295/5895 Three Dimensional Imaging of Materials
Guest lecturer
Slides available on request
Links:
http://www.engr.uconn.edu/me/cms/people/39-wilsonchiu (Website of Prof. Wilson K.S. Chiu (Course co-ordinator))

ISOS-7
Period: 7 Oct 2014
Michael Corazza (Speaker)
Department of Energy Conversion and Storage
Functional organic materials

Description
International Summit in OPV Stability (ISOS 7)
Links:
A Stability Study of Alkali Doped PBI Membranes for Alkaline Electrolyzer Cells
Jens Oluf Jensen (Invited speaker)
Department of Energy Conversion and Storage
Proton conductors

HIGH TEMPERATURE ALKALINE ELECTROLYSIS
Period: 2 Oct 2014
Christodoulos Chatzichristodoulou (Lecturer)
Department of Energy Conversion and Storage
Fundamental Electrochemistry
Documents:
HIGH TEMPERATURE ALKALINE ELECTROLYSIS_abstract

Er der vedvarende energi nok til os alle?: Om brændselsceller og elektrolyseceller til effektiv energikonvertering
Period: 26 Sep 2014
Anne Hauch (Lecturer)
Department of Energy Conversion and Storage
Applied Electrochemistry

Description
Foredrag i forbindelse med Dansk Naturvidenskabsfestival
Inviteret foredrag
Documents:
Brændselsceller_og_elektrolyseceller_DanskNaturvidenskabsfestival_AnneHauch_Sepa26th2014

Atomic-scale modeling in fuel cell, electrolyser and battery research; Transport modeling in batteries - ionic and electronic transport; Beyond Li-ion - resource-efficient batteries
Period: 22 Sep 2014 → 26 Sep 2014
Tejs Vegge (Invited speaker)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related event
JESS Summer School
22/09/2014 → 26/09/2014
Crete, Greece
Activity: Talks and presentations › Conference presentations

Massive scale production and installation of flexible printed solar cells
Period: 19 Sep 2014
Markus Hösel (Speaker)
Department of Energy Conversion and Storage
Functional organic materials

Related event
EOS Annual Meeting 2014 (EOSAM)
15/09/2014 → 19/09/2014
Berlin Adlershof, Germany
Activity: Talks and presentations › Conference presentations

Solid State Protonic Conductors - 17
Period: 14 Sep 2014 → 19 Sep 2014
Jens Oluf Jensen (Invited speaker)
Department of Energy Conversion and Storage
Proton conductors

Description
One great advantage of the most common fuel cells, the polymer based fuel cells, is the low operating temperature which allows for easy and fast start-up and a variety of materials for construction and sealing. However, over the years the interest for increasing the working temperature has been growing. The motivation is diverse. A slight increase above 100-120°C is desired by the automotive industry to ease thermal control. This has been attempted via optimization of the perfluorosulphonic acid based membranes. A further increase to 140-200°C is desired to increase the tolerance to CO and thus to ease the integration with a reformer for carbonaceous fuels. This has been achieved by the phosphoric acid doped polymer membranes like polybenzimidazole with the added benefit that water management is unnecessary. The next step in temperature could be to go above 230-250°C in order to utilize the waste heat for methanol steam reforming. This is most realistic with solid inorganic proton conductors or molten salts and phosphate systems like CsH2PO4 have proven promising. At even higher temperature reforming of dimethyl ether and after that ethanol should be possible. Another advantage of increased temperature might be that a candidate for replacing platinum as catalyst is more easily found. From the other end of the fuel cell temperature window solid oxide fuel cells are developing in the direction of lower operating temperatures from initially 1000°C to 600-700°C or even lower. The limiting factor is oxide ion conductivity, but which temperature would ultimately be the optimum if one could chose freely? The presentation will elaborate on the benefits of the different working temperatures based on simple system requirements with and without fuel reformers. Overall criteria are energy efficiency and system simplicity.


Related event
Solid State Protonic Conductors - 17
14/09/2014 → 19/12/2014
Seoul, Korea, Republic of
Activity: Talks and presentations › Conference presentations
Future Challenges for Room Temperature AMR Devices
Period: 10 Sep 2014
Kurt Engelbrecht (Keynote speaker)
Department of Energy Conversion and Storage
Electrofunctional materials

Related event
6th IIR/IIF International Conference on Magnetic Refrigeration
07/09/2014 → 10/09/2014
Victoria, Canada
Activity: Talks and presentations › Conference presentations

Microstructure analysis of vacuum plasma sprayed electrodes for alkaline electrolysis
Period: 10 Sep 2014
Jacob R. Bowen (Speaker)
Department of Energy Conversion and Storage
Imaging and Structural Analysis

Description
Oral presentation of abstract MS-14-O2142
Links:
http://www.imc2014.com (18th International Microscopy Congress website)

Related event
18th International Microscopy Congress 2014
07/09/2014 → 12/09/2014
Prague, Czech Republic
Activity: Talks and presentations › Conference presentations

Design and Initial Testing of a Compact and Efficient Rotary AMR Prototype
Period: 8 Sep 2014
Dan Eriksen (Speaker)
Department of Energy Conversion and Storage
Electrofunctional materials

Related event
6th IIR/IIF International Conference on Magnetic Refrigeration
07/09/2014 → 10/09/2014
Victoria, Canada
Activity: Talks and presentations › Conference presentations

6th IIR/IIF International Conference on Magnetic Refrigeration
Period: 7 Sep 2014 → 10 Sep 2014
Christian Bahl (Participant)
Department of Energy Conversion and Storage
Electrofunctional materials

Related event
6th IIR/IIF International Conference on Magnetic Refrigeration
07/09/2014 → 10/09/2014
Victoria, Canada
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.
**Description**

Presentation of a poster

International summer school on OPV

**Documents:**

Program summer school RHIN-SOLAR 2014

Poster_strasburg

**Related event**

International Summer School on OPV  
31/08/2014 → 04/09/2014  
Strasbourg, France

Activity: Talks and presentations › Guest lectures, external teaching and course activities at other universities

---

**DTU Energy Conversion 2nd International PhD Summer School**

**Period:** 29 Aug 2014

**Jacob R. Bowen (Participant)**

**Department of Energy Conversion and Storage**

**Imaging and Structural Analysis**

**Description**

The focused ion beam scanning electron microscope (FIB-SEM) is a versatile microscope that can be used for a wide range of applications including site specific transmission electron microscope (TEM) sample preparation, ion beam lithography, micro machining, integrated circuit edits, cross-sectioning and for serial sectioning to generate high resolution three dimensional images of microstructure. In the past decade the FIB-SEM has enabled many critical investigations of electrode microstructure to be performed. Electrodes tend to be made from heterogeneous stochastic porous composite materials that often have important nanoscale microstructure features. Making TEM samples to reveal critical local information from active sites within these electrodes is challenging. The FIB-SEM’s ability to make site specific samples regardless of material composition and hardness has been a major breakthrough for these devices. The FIB-SEM has also opened the door to nanometer resolution 3D imaging of electrode microstructures and provided access to for the first time microstructure parameters of electrodes only obtainable from 3D data. This talk will cover ion beam and FIB column basics, interactions of ions with materials for producing images and sputtering, ion and electron beam induced chemical vapour deposition, advantages and disadvantages of TEM sample preparation, practical aspects of serial sectioning for SEM imaging and electron backscatter diffraction (EBSD) from the users point of view. A series of examples of TEM sample preparation, 3D reconstructions and 3DEBSD on a range of energy materials will be presented as well as the range of information that can be extracted from 3D reconstructions of electrodes.

The Focused Ion Beam – Scanning Electron Microscope: A tool for sample preparation, two and three dimensional imaging

**Course lecturer**

**Documents:**

2014 IMAGINE FIB-SEM JR Bowen

**Links:**

https://files.conferencemanager.dk/medialibrary/010c1367-e991-4a33-ab10-1953247e9c23/images/2014_IMAGINE_FIB-SEM_JR_Bowen.pdf (Link to slides on summer school website)

http://www.conferencemanager.dk/IMAGINE/imagine.html (Summer school website)

**Related event**

**DTU Energy Conversion 2nd International PhD Summer School**
Kristine Munk Jespersen (Participant)

Department of Wind Energy
Composites and Materials Mechanics
Department of Energy Conversion and Storage

**Description**
Participation in DTU Energy Conversion 2nd International PhD Summer School along with poster presentation. The poster has been attached to this description.

**Documents:**
IMAGINE Poster by kmun

**Related event**

**DTU Energy Conversion 2nd International PhD Summer School: IMAGINE: Methods in Imaging of Energy Material Microstructure**
25/08/2014 → 29/08/2014
Hundested, Denmark
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

**DTU Energy Conversion 2nd International PhD Summer School**
Janet Jonna Bentzen (Participant)

Department of Energy Conversion and Storage
Imaging and Structural Analysis

**Documents:**
abstract_IMAGINE_jabe
IMAGINE_poster_jabe

**Related event**

**International Conference on SINTERING 2014**
Francesca Teocoli (Participant)

Department of Energy Conversion and Storage
Ceramic Engineering & Science

**Description**
SINTERING 2014 continues the series of sintering conferences which have previously been held in Pennsylvania, USA (1995, 1999, 2003), Grenoble, France (2005), California, USA (2008) and last time in Jeju, Korea (2011). The International Conference on SINTERING 2014 deals with the latest developments in the field of sintering. Advances in sintering theory, modelling and the sintering of all classes of powder materials from experimental to industrial scale are considered. We are looking forward to presentations and discussions in the following fields of expertise in particular • Fundamental Aspects of Sintering • Modelling and Simulation • Multi-Material Systems • Microstructure and Properties • Novel Sintering Processes • Sintering of Nano-structured Materials • Functional Materials • Chemical Interactions during Sintering • In-situ Measurement

**Documents:**
Abstract - Sintering2014
Links:
http://www.sintering2014.com

Related event

International Conference on SINTERING 2014
24/08/2014 → 28/08/2014
Dresden, Germany
Activity: Attending an event › Participating in or organising a conference

Magnetocaloric Cooling and Heating
Period: 22 Aug 2014
Søren Linderoth (Lecturer)
Department of Energy Conversion and Storage
Description
Invited to Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Science
Documents:
Prof Linderoth-Poster

Related event

Seminar at Beijing National Laboratory for Condensed Matter Physics, Institute of Physics, Chinese Academy of Science
22/08/2014 → …
Beijing, China
Activity: Talks and presentations › Conference presentations

Academic research in higher education
Period: 20 Aug 2014
Duc-The Ngo (Invited speaker)
Department of Energy Conversion and Storage
Imaging and Structural Analysis
Department of Micro- and Nanotechnology
Molecular Windows
Description
A keynote lecture at Vietnam Summer School of Science
Vietnam Summer School of Science

Related external organisation

Unknown external organisation
Activity: Talks and presentations › Conference presentations

5th International Conference on Ceramics
Søren Linderoth (Keynote speaker)
Department of Energy Conversion and Storage
Description
Professor Søren Linderoth was a key note speaker at the ICC5 in Beijing, China, August 2014

Related event

5th International Conference on Ceramics: ICC5
18/08/2014 → 22/08/2014
Beijing, China
Activity: Talks and presentations › Conference presentations

2014 CAMD Summer School on Electronic Structure Theory and Materials Design
Rune Christensen (Participant)
Department of Energy Conversion and Storage
Atomic scale modelling and materials
Theoretical Atomic-scale Physics

Description
CAMD Summer School

Related event

2014 CAMD Summer School on Electronic Structure Theory and Materials Design
17/08/2014 → 23/08/2014
Lyngby, Denmark
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Electrochemical Energy Storage and Electrofuels
Tejs Vegge (Invited speaker)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related event

2014 CAMD Summer School on Electronic Structure Theory and Materials Design
17/08/2014 → 23/08/2014
Lyngby, Denmark
Activity: Talks and presentations › Conference presentations

14th International Symposium on Metal-Hydrogen Systems: Fundamentals and Applications
Period: 22 Jul 2014
Didier Blanchard (Participant)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Description
Poster presentation - A Class of Superior Ammonia Storage Materials Based on Solid Solution of Barium Strontium Chloride Salts Got a poster awards

Poster presentation

Related event

14th International Symposium on Metal-Hydrogen Systems: Fundamentals and Applications
20/07/2014 → 25/07/2014
Manchester, United Kingdom
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Board Committee Member of The International Academy of Electrochemical Energy Science (External organisation)
Period: 14 Jul 2014 → 14 Jul 2017
Qingfeng Li (Participant)
Department of Energy Conversion and Storage
Proton conductors

**Description**
The International Academy of Electrochemical Energy Science

Body type: an international organization
Degree of recognition: International

**Related external organisation**

*Board Committee Member of The International Academy of Electrochemical Energy Science*
Activity: Membership › Membership of committees, commissions, boards, councils, associations, organisations, or similar

**13th International Conference Inorganic Membranes**
Period: 8 Jul 2014
Shiyang Cheng (Speaker)
Department of Energy Conversion and Storage
Mixed Conductors

**Description**
Best student poster award

**Related event**

*13th International Conference Inorganic Membranes*
06/07/2012 → 09/07/2014
Brisbane, Australia
Activity: Talks and presentations › Conference presentations

**Overview of SOFC/SOEC development at DTU Energy Conversion**
Period: 2 Jul 2014
Anke Hagen (Lecturer)
Department of Energy Conversion and Storage
Applied Electrochemistry

**Related event**

*European fuel cell 2014 - 11th European SOFC and SOE Forum 2014*
01/07/2014 → 04/07/2014
Lucerne, Switzerland
Activity: Talks and presentations › Conference presentations

**Designing Nanoparticle Electrocatalysts for Sustainable Production of Synthetic Fuels**
Period: 1 Jul 2014 → 3 Jul 2014
Tejs Vegge (Invited speaker)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials

**Related event**

*QuantumHagen: Workshop on Modeling of Electronic Devices and Materials at the Nanoscale*
01/07/2014 → 03/07/2014
Copenhagen, Denmark
Activity: Talks and presentations › Conference presentations
**European fuel cell 2014 - 11th European SOFC and SOE Forum 2014**

Period: 1 Jul 2014 → 4 Jul 2014

Benoit Charlas (Participant)

Department of Energy Conversion and Storage

**Mixed Conductors**

**Description**

Poster B1107 - Residual stresses in a co-sintered SOC half-cell during post-sintering cooling

**European Fuel cell forum 2014**

**Related event**

**European fuel cell 2014 - 11th European SOFC and SOE Forum 2014**

01/07/2014 → 04/07/2014

Lucerne, Switzerland

Activity: Attending an event › Participating in or organising a conference

**Anne Hauch (Speaker)**

Department of Energy Conversion and Storage

**Applied Electrochemistry**

**Description**

"Ni/YSZ microstructure optimization for long-term stability of solid oxide electrolysis cells" (presentation)

**Related event**

**European fuel cell 2014 - 11th European SOFC and SOE Forum 2014**

01/07/2014 → 04/07/2014

Lucerne, Switzerland

Activity: Talks and presentations › Conference presentations

**Simon Loftager (Participant)**

Center for Atomic-scale Materials Design

Department of Energy Conversion and Storage

**Atomic scale modelling and materials**

**Related event**

**QuantumWise Workshop**

Period: 1 Jul 2014 → 3 Jul 2014

København, Denmark

Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.


Period: Jun 2014

Ngo Van Nong (Chairman)

Department of Energy Conversion and Storage

**Electrofunctional materials**

**Description**

Oxide devices: thermoelectric conversion, Resistive sensors, spintronics, and superconductors
Related event

10/06/2014 → …
Taipei, Taiwan, Province of China
Activity: Attending an event › Participating in or organising a conference

IUMRS-ICEM 2014
Period: Jun 2014
Ngo Van Nong (Invited speaker)
Department of Energy Conversion and Storage
Electrofunctional materials

Description
Thermoelectric oxides for effective power generation from high temperature waste heat

Related external organisation

Unknown external organisation
Activity: Talks and presentations › Conference presentations

International Conference on Synthetic Metal
Period: 30 Jun 2014 → 5 Jul 2014
Emil Beje Lind Pedersen (Speaker)
Department of Energy Conversion and Storage
Imaging and Structural Analysis

Description
Participated with a talk titled: “Characterization of organic water dispersible nanoparticles useable in photovoltaics”

Talk at ICSM 2014 (International Conference on Synthetic Metals)

Related event

International Conference on Synthetic Metal: Synthetic Metals Guiding the Future
30/06/2014 → 05/07/2014
Turku, Finland
Activity: Talks and presentations › Conference presentations

In situ and operando X-ray absorption spectroscopy on SOFC materials and cells
Period: 27 Jun 2014
Anke Hagen (Lecturer)
Department of Energy Conversion and Storage
Applied Electrochemistry

Related event

Challenges and Opportunities in In Situ Studies of Solid Oxide Electrodes
26/06/2014 → 27/06/2014
Risø, Denmark
Activity: Talks and presentations › Conference presentations

ASME 2014 12th Biennial Conference on Engineering Systems Design and Analysis
Kurt Engelbrecht (Organizer)
Department of Energy Conversion and Storage
Electrofunctional materials
Description
Track co-leader Heat Transfer and Thermal Engineering

Session chair: Numerical Applications 1
Gave presentation: "Modelling and Simulation of Regenerators With Complex Flow Arrangements for Active Magnetocaloric Refrigeration"

Related event

**ASME 2014 12th Biennial Conference on Engineering Systems Design and Analysis**
25/06/2014 → 27/06/2014
Copenhagen, Denmark
Activity: Attending an event › Participating in or organising a conference

**Computational Search for Improved Ammonia Storage Materials**
Period: 19 Jun 2014
Peter Bjerre Jensen (Lecturer)
Atomic scale modelling and materials
Department of Energy Conversion and Storage
Center for Atomic-scale Materials Design
Department of Physics
Documents:
abstract

Related event

**CIMTEC 2014: 6th Forum on New Materials**
15/06/2014 → 19/06/2014
Montecatini Terme, Italy
Activity: Talks and presentations › Conference presentations

**CIMTEC 2014**
Period: 18 Jun 2014
Didier Blanchard (Speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Description
Presentation title: Mixed Metal Ammine Complexes for Hydrogen/NH3 Storage

Oral presentation

Related event

**CIMTEC 2014: 6th Forum on New Materials**
15/06/2014 → 19/06/2014
Montecatini Terme, Italy
Activity: Talks and presentations › Conference presentations

**Materials Predictors and Genetic Algorithms for Rational Design of Electrocatalytic Nanoclusters**
Period: 16 Jun 2014 → 21 Jun 2014
Tejs Vegge (Invited speaker)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related event
Clusters 2014
16/06/2014 → 21/06/2014
Aalto, Finland
Activity: Talks and presentations › Conference presentations

20th World Hydrogen Energy Conference 2014
Period: 15 Jun 2014 → 20 Jun 2014
Jens Oluf Jensen (Speaker)
Department of Energy Conversion and Storage
Proton conductors

Description

Related event
20th World Hydrogen Energy Conference 2014
15/06/2014 → 20/06/2014
Gwangju Metropolitan City, Korea, Republic of
Activity: Talks and presentations › Conference presentations

Danscatt Annual Meeting 2014
Period: 22 May 2014 → 23 May 2014
Emil Bøje Lind Pedersen (Speaker)
Imaging and Structural Analysis
Department of Energy Conversion and Storage

Description
Presented a poster titled: "X-ray study of organic nanoparticles for plastic solar cells"

Participation in "Danscatt Annual Meeting 2014"

Related event
Danscatt Annual Meeting 2014
22/05/2014 → 23/05/2014
Lyngby, Denmark
Activity: Talks and presentations › Conference presentations

Designing New Materials for Ammonia Storage Using Density Functional Theory and Genetic Algorithms
Period: 14 May 2014
Peter Bjerre Jensen (Lecturer)
Department of Energy Conversion and Storage
Center for Atomic-scale Materials Design
Atomic scale modelling and materials
Documents:
A-O- 099 - Jensen Peter Bjerre

Related event
International Discussion on Hydrogen Energy and Applications
12/05/2014 → 14/05/2014
Nantes, France
Activity: Talks and presentations › Conference presentations
QENS 2014 / WINS 2014
Period: 13 May 2014
Didier Blanchard (Speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Description
Presentation title: Li-ion conduction in the LiBH4:LiI system from density functional theory calculations and quasi-elastic neutron scattering

Oral Presentation

Related event

QENS 2014 / WINS 2014
11/05/2014 → 16/05/2014
Autrans, France
Activity: Talks and presentations › Conference presentations

Will organic photovoltaic technology render benefits in a near future of a 30 years horizon?
Period: 12 May 2014
Nieves Espinosa Martinez (Lecturer)
Department of Energy Conversion and Storage
Functional organic materials

Related event

SETAC Europe 24th Annual Meeting
11/05/2014 → 15/05/2014
Basel, Switzerland
Activity: Talks and presentations › Conference presentations

Brændselsceller og elektrolyse: En del af løsningen for fremtidens energiudfordringer
Period: Apr 2014
Anke Hagen (Invited speaker)
Department of Energy Conversion and Storage
Applied Electrochemistry

Description
Four public presentations: Roskilde Gymnasium, Helsingør Technical Museum, Kirke Helsinge Skole, Nordstjerneskolen Helsinge

Related event

Bestil en Forsker - Forskningens Døgn
24/04/2014 → 26/04/2014
Denmark
Activity: Talks and presentations › Conference presentations

Forskningens Døgn 2014
Period: Apr 2014
Anke Hagen (Organizer)
Department of Energy Conversion and Storage
Applied Electrochemistry

Related event

Forskningens Døgn 2014
Infinitely Large Organic Solar Cell Modules: At The Edge Of Traditional Territories For Power Supply
Period: 16 Apr 2014
Nieves Espinosa Martinez (Invited speaker)
Department of Energy Conversion and Storage
Functional organic materials

Related event
2nd International Conference on Clean Energy
13/04/2014 → 16/04/2014
Qingdao, China
Activity: Talks and presentations › Conference presentations

Fully printed multi square meter large organic solar cell modules for real energy production
Period: 15 Apr 2014
Markus Hösel (Speaker)
Department of Energy Conversion and Storage
Functional organic materials

Related event
2nd International Conference on Clean Energy
13/04/2014 → 16/04/2014
Qingdao, China
Activity: Talks and presentations › Conference presentations

Outdoor Operational Stability of Indium-free Polymer Solar Cell Modules Investigated over 1 year
Period: 15 Apr 2014
Dechan Angmo (Speaker)
Department of Energy Conversion and Storage
Functional organic materials

Related event
2nd International Conference on Clean Energy
13/04/2014 → 16/04/2014
Qingdao, China
Activity: Talks and presentations › Conference presentations

IRENA Workshop - The Transformative Power of Storage: Developing IRENA’s Electricity Storage Roadmap
Period: 27 Mar 2014
Allan Schroeder Pedersen (Lecturer)
Department of Energy Conversion and Storage

Description
An overview of energy storage technology development roadmap work done in a European and Danish perspective was given. Presentation given in collaboration with Energinet.dk.

Related event
IRENA Workshop: The Transformative Power of Storage: Developing IRENA's Electricity Storage Roadmap
27/03/2014 → …
Düsseldorf, Denmark
Activity: Talks and presentations › Conference presentations
What is a solar cell
Period: 27 Mar 2014
Michael Corazza (Lecturer)
Department of Energy Conversion and Storage
Functional organic materials
Documents:
Program 27 3 HTX Roskilde- intro
What is a Solar Cell_v3

Related event
High school talk
27/03/2014 → 27/03/2014
Denmark
Activity: Talks and presentations › Conference presentations

Department of Energy Conversion and Storage-Solid Oxide Fuel and Electrolysis Cells
Period: 12 Mar 2014
Anke Hagen (Invited speaker)
Department of Energy Conversion and Storage
Applied Electrochemistry

Related event
Department of Energy Conversion and Storage-Solid Oxide Fuel and Electrolysis Cells
12/03/2014 → …
Lund, Sweden
Activity: Talks and presentations › Conference presentations

Dansk energisystem uden fossile brændsler – er det muligt?
Period: 6 Mar 2014
Søren Linderoth (Speaker)
Department of Energy Conversion and Storage

Related event
Møde i UNF København (Ungdommens Naturvidenskabelige Forening)
06/03/2014 → …
København, Denmark
Activity: Talks and presentations › Conference presentations

Computational of Nanoparticle Catalysts for Sustainable Production of Synthetic Fuels
Period: 16 Feb 2014 → 21 Feb 2014
Tejs Vegge (Invited speaker)
Center for Atomic-scale Materials Design
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related event
8th International Symposium Hydrogen and Energy
16/02/2014 → 21/02/2014
Zhaoqing, China
Activity: Talks and presentations › Conference presentations
High resolution ptychographic tomography of soft matter
Period: 30 Jan 2014
Jens Wenzel Andreasen (Invited speaker)
Department of Energy Conversion and Storage
Imaging and Structural Analysis
Links:
https://indico.desy.de/getFile.py/access?resId=47&amp;materialId=0&amp;confId=9088 (Programme)

Related event
4th Workshop on X-Ray Nano-Imaging of Biological and Chemical Systems at PETRA III: DESY Photon Science Users' Meeting
29/01/2014 → 31/01/2014
Hamburg, Germany
Activity: Talks and presentations › Conference presentations

Mechanical Properties of Ceramics and Glass
Period: 30 Jan 2014 → 31 Jan 2014
Francesca Teocoli (Participant)
Department of Energy Conversion and Storage
Ceramic Engineering & Science
Description
Short Course: Mechanical Properties of Ceramics and Glass. Instructors: Richard C. Bradt, University of Alabama, and George Quinn, NIST
Participation to the short course on "Mechanical Properties of Ceramics and Glass".

Related event
Mechanical Properties of Ceramics and Glass
30/01/2014 → 31/01/2014
Daytona Beach - Florida, United States
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

38th International Conference and Expo on Advanced Ceramics and Composites
Period: 26 Jan 2014 → 31 Jan 2014
Vincenzo Esposito (Organizer)
Department of Energy Conversion and Storage
Ceramic Engineering & Science
Description
11th International Symposium on Solid Oxide Fuel Cells (SOFC): Materials, Science and Technology
38th International Conference and Expo on Advanced Ceramics and Composites
Links:

Related event
38th International Conference and Expo on Advanced Ceramics and Composites
26/01/2014 → 31/01/2014
Daytona Beach, FL, United States
Activity: Attending an event › Participating in or organising a conference
Thermo-mechanical properties of SOFC components investigated by a combined method
Period: 26 Jan 2014
Francesca Teocoli (Speaker)
Department of Energy Conversion and Storage
Ceramic Engineering & Science
Documents:
Abstract_ICACC14_Teocoli_Francesca

Related event
38th International Conference and Exposition on Advanced Ceramics and Composites
26/01/2014 → 31/01/2014
Daytona Beach, FL, United States
Activity: Talks and presentations › Conference presentations

Eurotech participants meeting
Period: 23 Jan 2014
Michael Corazza (Speaker)
Department of Energy Conversion and Storage
Functional organic materials
Documents:
140124 - EuroTech - Summary

Related event
Eurotech participants meeting
23/01/2014 → 24/01/2014
Neuchatel, Switzerland
Activity: Talks and presentations › Conference presentations

Chemical Vapour Deposition: CVD of Tantalum
Period: 2013
James Atwoki Mugabi (Other)
Department of Energy Conversion and Storage
Proton conductors
Description
Part of the course - Ceramic Science and Engineering (1st lecture in spring 2013 and 2nd lecture in spring 2014)

Related event
Ceramic Science and Engineering
01/02/2013 → …
Denmark
Activity: Talks and presentations › Conference presentations

Delft Days on Magnetocalorics (2013)
Period: 2013
Henrique Neves Bez (Participant)
Department of Energy Conversion and Storage
Electrofunctional materials
Description
Poster presentation on the preparation of magnetocaloric perovskite.

Related event
Delft Days on Magnetocalorics (2013)
28/10/2013 → 29/10/2013
Delft, Netherlands
Activity: Attending an event › Participating in or organising a conference

**Elchemea Analytical: Software til impedans-analyse**
*Period:* 2013
*Søren Koch (Participant)*
Department of Energy Conversion and Storage
Applied Electrochemistry

**Description**
Open source software offentliggjort under GPL
*Head:* Søren Koch
*Links:* http://www.elchemea.com
*Activity:* Other

**Light trapping with plasmonic oligomers and photonic crystals to enhance the performance of organic solar cells devices**
*Period:* 2013 → …
*Francesco Pastorelli (Speaker)*
Department of Energy Conversion and Storage
Functional organic materials

**Related event**

**Complex nanophotonics**
27/08/2013 → 31/08/2013
London, United Kingdom
*Activity:* Talks and presentations › Conference presentations

**Plasmonic Oligomers studies to Enhance the Performance of Organic Solar Cells devices**
*Period:* 2013 → …
*Francesco Pastorelli (Speaker)*
Department of Energy Conversion and Storage
Functional organic materials

**Related event**

**Plasmonica 2013**
01/07/2013 → 03/07/2013
Milano, Italy
*Activity:* Talks and presentations › Conference presentations

**Topical meeting on "Dispersion and Interface chemistry" in the Danish Ceramic Society**
*Period:* 18 Dec 2013
*Micela Della Negra (Invited speaker)*
Department of Energy Conversion and Storage
Ceramic Engineering & Science

**Description**
Stability studies on ceramic suspensions using complementary analysis techniques.

**Related event**

**Topical meeting on "Dispersion and Interface chemistry" in the Danish Ceramic Society**
Microstructure characterisation of solid oxide electrolysis cells operated at high current density

Period: 6 Dec 2013
Jacob R. Bowen (Invited speaker)

Imaging and Structural Analysis

Department of Energy Conversion and Storage

Description

High temperature solid oxide cells can be operated either as fuel cells or electrolysis cells for efficient power generation or production of hydrogen from steam or synthesis gas (H2 + CO) from steam and CO2 respectively. When operated under harsh conditions, they often exhibit microstructural degradation of cell components in relation to the loss of electrochemical performance specific to the mode of operation. Thus descriptive microstructure characterization methods are required in combination with electrochemical characterization methods to decipher degradation mechanisms. In the present work, microstructure evolution of the Ni-yttria stabilized zirconia (YSZ) is followed as a function of galvanostatic steam electrolysis testing at current densities between -0.5 and -1.0 A cm-2 for periods of up to 750 hours at 800 °C. The volume fraction and size of the percolating Ni particles was statistically quantified using the mean linear intercept method as a function of current density and correlated to increases in serial resistance. The above structural changes are then compared in terms of electrode degradation observed during the co-electrolysis of steam and CO2 at current densities up to -1.5 A cm-2. In this study, the formation of ZrO2 based nano particles at the Ni-pore interface is responsible for the loss of Ni-YSZ particle contact and thus loss of triple phase boundary. Formation of similar nano particles at Ni internal grain boundaries is also thought to be responsible for loss of Ni percolation.

Related event

Thermec 2013 - International Conference on Processing & Manufacturing of Advanced Materials: Processing, Fabrication, Properties, Application
02/12/2013 → 06/12/2013
Las Vegas, United States

Activity: Talks and presentations › Conference presentations

Combined computational and experimental study of the role of CO2 poisoning on the electronic conduction and overpotentials in Li-air batteries

Period: 4 Dec 2013 → 5 Dec 2013
Tejs Vegge (Invited speaker)

Department of Energy Conversion and Storage

Atomic scale modelling and materials

Related event

Nordisk Batterikonferens 2013 (NORDBATT)
04/12/2013 → 05/12/2013
Uppsala, Sweden

Activity: Talks and presentations › Conference presentations

Electrospin our Energy Devices

Period: 3 Dec 2013

Wenjing (Angela) Zhang (Invited speaker)

Department of Energy Conversion and Storage

Ceramic Engineering & Science

Documents:
Invitation letter for Dr W Zhang

Related event

Electrospin Our Energy Devices
03/12/2013 → …
Adelaide, Australia
Activity: Talks and presentations › Conference presentations

**Shaping our Energy Future with Electrospinning**  
*Period: 2 Dec 2013*  
*Wenjing (Angela) Zhang (Invited speaker)*  
*Department of Energy Conversion and Storage*  
*Ceramic Engineering & Science*

**Description**  
Invited speaker for Research Seminar in School of Chemical Engineering at The University of Adelaide.

**Documents:**  
Seminar Abstract_20131202

**Related event**  
*School of Chemical Engineering Research Seminar*  
*02/12/2013 → …*  
*Adelaide, Australia*  
*Activity: Talks and presentations › Conference presentations*

**the 10th International Symposium on Novel Carbon Resource Sciences**  
*Period: 2 Dec 2013*  
*Ngo Van Nong (Lecturer)*  
*Department of Energy Conversion and Storage*  
*Electrofunctional materials*

**Related external organisation**  
*Unknown external organisation*  
*Activity: Talks and presentations › Conference presentations*

**2013 MRS Fall Meeting & Exhibit**  
*Period: 1 Dec 2013 → 6 Dec 2013*  
*Thanh Hung Le (Participant)*  
*Department of Energy Conversion and Storage*  
*Electrofunctional materials*

**Documents:**  
MRS_Abstract

**Related event**  
*2013 MRS Fall Meeting & Exhibit*  
*01/12/2013 → 06/12/2013*  
*Boston, MA, United States*  
*Activity: Attending an event › Participating in or organising a conference*

**Design of Experiment**  
*Period: 26 Nov 2013 → 27 Nov 2013*  
*Francesca Teocoli (Participant)*  
*Department of Energy Conversion and Storage*  
*Ceramic Engineering & Science*

**Description**  
Short Course: Design of Experiments. Instructors: Jakob Christensen, Umetric AB, Umeå, Sweden.

Participation to the short course on "Design of Experiments".
Related event

Design of Experiment
26/11/2013 → 27/11/2013
Roskilde, Denmark
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

3-Dimensional Nanofiber Electrodes for Solid Oxide Fuel Cells and Proton Exchange Membrane Fuel Cells
Period: 25 Nov 2013
Wenjing (Angela) Zhang (Lecturer)
Department of Energy Conversion and Storage
Ceramic Engineering & Science

Related event

3-Dimensional Nanofiber Electrodes for Solid Oxide Fuel Cells and Proton Exchange Membrane Fuel Cells
25/11/2013 → …
Melbourne, Australia
Activity: Talks and presentations › Conference presentations

Sustainable Fuels from Renewable Energies
Period: 20 Nov 2013
Mogens Bjerg Mogensen (Invited speaker)
Department of Energy Conversion and Storage
Fundamental Electrochemistry

Description
Electrolysis for conversion of H2O and CO2 into green fuels.

Related event

Sustainable Fuels from Renewable Energies: IASS Brainstorming Workshop
19/11/2013 → 20/11/2013
Potsdam, Germany
Activity: Talks and presentations › Conference presentations

Electrochemical Energy Storage - Batteries
Period: 14 Nov 2013
Tejs Vegge (Invited speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related event

DTU International Energy Report 2013 Symposium
14/11/2013 → …
Lyngby, Denmark
Activity: Talks and presentations › Conference presentations

ENHANCED MASS DIFFUSION PHENOMENA IN HIGHLY DEFECTIVE DOPED CERIA: LIMITS AND APPLICATIONS:
Ionic and Electronic Conductors and Applications to Solid Oxide Fuel Cells and Membrane Technology
Period: 13 Nov 2013
Vincenzo Esposito (Invited speaker)
Department of Energy Conversion and Storage
Ceramic Engineering & Science
Documents:
ICE2013-VIES_GDC enhanched
Related event

6th International Conference on Electroceramics
09/11/2013 → 13/11/2013
João Pessoa, Brazil
Activity: Talks and presentations › Conference presentations

DTU Energy Conversion PhD symposium 2013
Period: 8 Nov 2013
Thanh Hung Le (Participant)
Department of Energy Conversion and Storage
Electrofunctional materials

Description
High-temperature thermoelectric oxide modules for effective power generation from waste heat.
Links:
http://www.ecs.dtu.dk/Kalender/2013/11/PhD-symposium

Related event

DTU Energy Conversion PhD symposium 2013
08/11/2013 → 08/11/2013
Roskilde, Denmark
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Første symposium hos Institut for Energikonvertering- og lagring
Period: 8 Nov 2013
Simon Loftager (Participant)
Center for Atomic-scale Materials Design
Department of Physics
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related event

Første symposium hos Institut for Energikonvertering- og lagring
08/11/2013 → 08/11/2013
Roskilde, Denmark
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Period: 3 Nov 2013 → 6 Nov 2013
Ngo Van Nong (Invited speaker)
Department of Energy Conversion and Storage
Electrofunctional materials

Description
Plenary talk

Related external organisation

Unknown external organisation
Activity: Talks and presentations › Conference presentations
**Delft Days on Magnetocalorics (2013)**
Lars von Moos (Participant)
Department of Energy Conversion and Storage
Electrofunctional materials

**Description**
Participant and poster presenter

Delft Days on Magnetocalorics 2013.
Documents:
Lars_von_Moos_PosterDDMC13

**Related event**

Delft Days on Magnetocalorics (2013)
28/10/2013 → 29/10/2013
Delft, Netherlands
Activity: Attending an event › Participating in or organising a conference

**Calculational and experimental study of the role of CO2 poisoning on the electronic conduction and overpotentials in Li-air batteries**
Tejs Vegge (Speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

**Related event**

224th Electrochemical Society Meeting
27/10/2013 → 01/11/2013
San Francisco, CA, United States
Activity: Talks and presentations › Conference presentations

**Design and optimisation of permanent magnet systems for magnetic refrigeration**
Period: 25 Oct 2013
Christian Bahl (Lecturer)
Department of Energy Conversion and Storage
Electrofunctional materials

**Related event**

Applied Magnetic Materials
24/10/2013 → 25/10/2013
Pori, Finland
Activity: Talks and presentations › Conference presentations

**13th International Symposium on Solid Oxide Fuel Cells (SOFC-XIII)**
Anne Hauch (Participant)
Applied Electrochemistry
Department of Energy Conversion and Storage

**Description**
 Participation in and oral presentation at the 13th International Symposium on Solid Oxide Fuel cells (SOFC-XIII)

Sulfur Poisoning of Ni/stabilized-zirconia Anodes – Effect on Long-Term Durability
The Danish Energy Agreement and Solid Oxide Cells
Period: 6 Oct 2013
Anke Hagen (Lecturer)
Department of Energy Conversion and Storage
Applied Electrochemistry

Smart Energy Conversion and Storage Conference
Period: 2 Oct 2013
Mogens Bjerg Mogensen (Invited speaker)
Department of Energy Conversion and Storage
Fundamental Electrochemistry

Description
Current Density - Overvoltage Relations for Solid Oxide Electrodes.
Invited Talk at "Smart Energy Conversion and Storage Conference".

Smart Energy Conversion and Storage Conference: IV Polish Forum
Period: 30 Sep 2013
Lars von Moos (Speaker)
Department of Energy Conversion and Storage
Electrofunctional materials

Description
North Carolina State University.

Related external organisation
Unknown external organisation
Activity: Talks and presentations › Conference presentations

Computational screening of mixed metal halide ammines
Period: 17 Sep 2013
Peter Bjerre Jensen (Lecturer)
Department of Energy Conversion and Storage
Atomic scale modelling and materials
Related event

E-MRS 2013 Fall Meeting. Symposium C
16/09/2013 → 20/09/2013
Warsaw, Poland
Activity: Talks and presentations › Conference presentations

From magnetocaloric materials to magnetic refrigeration devices
Period: 10 Sep 2013
Christian Bahl (Invited speaker)
Department of Energy Conversion and Storage
Electrofunctional materials

Related event

Donostia International Conference on Nanoscaled Magnetism and Applications
09/09/2013 → 13/12/2013
San Sebastian, Spain
Activity: Talks and presentations › Conference presentations

Electrochemical reduction of CO2 and H2O into fuels: Cell types and kinetic barriers
Period: 9 Sep 2013
Mogens Bjerg Mogensen (Keynote speaker)
Department of Energy Conversion and Storage
Fundamental Electrochemistry

Related event

246th American Chemical Society National Meeting : Symposium on "Electrocatalysis of Energy Generation and Storage"
08/09/2013 → 12/09/2013
Indianapolis, United States
Activity: Talks and presentations › Conference presentations

Functional dependent errors in DFT calculations for Li-air batteries
Period: 9 Sep 2013
Rune Christensen (Speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials
Center for Atomic-scale Materials Design
Department of Physics

Description
Presentation of key conclusions from Masters thesis.

Related event

2nd ReLiable Li-Air Workshop
09/09/2013 → 10/09/2013
Copenhagen, Denmark
Activity: Talks and presentations › Conference presentations

Materials Predictors and Genetic Algorithms for Design of Nanoparticle Activity and Stability
Period: 3 Sep 2013 → 7 Sep 2013
Tejs Vegge (Invited speaker)
Department of Energy Conversion and Storage

Atomic scale modelling and materials

Related event

International Conference on Computational Modelling of Nanostructured materials, ICCNM 2013
03/09/2013 → 07/09/2013
Frankfurt am Main, Germany
Activity: Talks and presentations › Conference presentations

1st International PhD Summer School
Period: 28 Aug 2013
Jacob R. Bowen (Lecturer)
Department of Energy Conversion and Storage
Imaging and Structural Analysis

Description
Microscopy methods for advanced ceramics
Course lecturer

Related event

1st International PhD Summer School: Optimized Processing of Multi-material Architectures for Functional Ceramics
26/08/2013 → 31/08/2013
Roskilde, Denmark
Activity: Talks and presentations › Guest lectures, external teaching and course activities at other universities

1st Workshop in Prof. John Irvine's EPSRC Platform project
Period: 28 Aug 2013
Mogens Bjerg Mogensen (Invited speaker)
Department of Energy Conversion and Storage
Fundamental Electrochemistry

Description
Title: Reversible oxide cells: Visions, limitations and possibilities.

Participated as member of the advisory committee of Prof. John Irvine's (St. Andrews University, Scotland) EPSRC Platform project, and gave an invited talk.

Related event

1st Workshop in Prof. John Irvine's EPSRC Platform project
27/08/2013 → 28/08/2013
Aviemore, Scotland, United Kingdom
Activity: Talks and presentations › Conference presentations

1st International PhD Summer School
Period: 26 Aug 2013 → 31 Aug 2013
Francesca Teocoli (Participant)
Department of Energy Conversion and Storage
Ceramic Engineering & Science

Related event

1st International PhD Summer School: Optimized Processing of Multi-material Architectures for Functional Ceramics
26/08/2013 → 31/08/2013
Roskilde, Denmark
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.
1st PhD summer school  
Period: 26 Aug 2013 → 30 Aug 2013  
Thanh Hung Le (Participant)  
Department of Energy Conversion and Storage  
Electrofunctional materials  
Documents:  
PhD_summer_school_Thanh_Hung_Le_Abstract  
Links:  
http://indico.conferences.dtu.dk/conferenceDisplay.py?ovw=True&confId=130  

Related event  
1st PhD summer school  
26/08/2013 → 30/08/2013  
Roskilde, Denmark  
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.  

The challenges in going from magnetocaloric materials to magnetic refrigeration devices  
Period: 29 Jul 2013  
Christian Bahl (Invited speaker)  
Department of Energy Conversion and Storage  
Electrofunctional materials  
Related event  
SPP 1599 Convention  
29/07/2013 → 01/08/2013  
Lichtenfels, Germany  
Activity: Talks and presentations › Conference presentations  

Eurotech participants meeting  
Period: 17 Jul 2013  
Michael Corazza (Speaker)  
Department of Energy Conversion and Storage  
Functional organic materials  
Description  
Eurotech participants meeting  
Related event  
Eurotech participants meeting  
17/07/2013 → 18/07/2013  
Munich, Germany  
Activity: Talks and presentations › Conference presentations  

Solid Oxide Fuel Cell Promise, Progress, and Priorities Workshop  
Period: 11 Jul 2013  
Mogens Bjerg Mogensen (Invited speaker)  
Department of Energy Conversion and Storage  
Fundamental Electrochemistry  
Description  
SOFC Funding Assessment Committee Contribution A presentation about possible strategies based on my long experience inside the area of SOFC R&D.  
Solid Oxide Fuel Cell Promise, Progress, and Priorities Workshop.
A workshop on solid oxide fuel cell R&D strategies.

Related event

**Solid Oxide Fuel Cell Promise, Progress, and Priorities Workshop**
Period: 11/07/2013 → 12/07/2013
Arlington, United States
Activity: Talks and presentations › Conference presentations

32nd International Conference on Thermoelectrics
Period: 30 Jun 2013 → 4 Jul 2013
Kobe, Japan
Activity: Attending an event › Participating in or organising a conference

Materials for energy storage – screening and evolution
Period: 25 Jun 2013 → 30 Jun 2013
Reykjavik, Iceland
Activity: Talks and presentations › Conference presentations

Computationa screening and design of energy materials – navigating vast phase spaces
Period: 24 Jun 2013 → 28 Jun 2013
Reykjavik, Iceland
Activity: Talks and presentations › Conference presentations

Arthur S. Nowick Memorial Symposium
Period: 7 Jun 2013
Stanford, United States
Activity: Talks and presentations › Conference presentations

Description
Invited presentation: Volume of Oxide Vacancies in Fluorite and Perovskite Structured Oxides.

Invited participant in Arthur S. Nowick Memorial Symposium.

Related event

Arthur S. Nowick Memorial Symposium
07/06/2013 → …
Kyoto, Japan
Activity: Talks and presentations › Conference presentations

Reversible solid oxide cells: limitations and possibilities
Period: 4 Jun 2013
Mogens Bjerg Mogensen (Invited speaker)
Department of Energy Conversion and Storage
Fundamental Electrochemistry

Description
Invited presentation at and participation in 19th International Conference on Solid State Ionics. Documents:
\ri-filab\home\momo\My Documents\Conferences and meetings\SSI-19\REVERSIBLE SOLID OXIDE CELLS LIMITATIONS AND POSSIBILITIES\SSI-19_Abstract_Invited_Mogens

Related event

19th International Conference on Solid State Ionics
02/06/2013 → 07/06/2013
Kyoto, Japan
Activity: Talks and presentations › Conference presentations

10th Pacific Rim Conference on Ceramic and Glass Technology
Period: 2 Jun 2013 → 7 Jun 2013
Francesca Teocoli (Participant)
Department of Energy Conversion and Storage
Ceramic Engineering & Science

Description
Poster presentation.
Documents:
Abstract_PACRIM10_Teocoli_Francesca

Related event

10th Pacific Rim Conference on Ceramic and Glass Technology
02/06/2013 → 07/06/2013
San Diego, CA, United States
Activity: Attending an event › Participating in or organising a conference

Sintering of Ceramics
Period: 1 Jun 2013 → 2 Jun 2013
Francesca Teocoli (Participant)
Department of Energy Conversion and Storage
Ceramic Engineering & Science

Description
Short Course: Sintering of Ceramics. Instructors: Mohamed N. Rahaman, Missouri University of Science and Technology.
Participation to the short course on "Sintering of Ceramics".
Related event

Sintering of Ceramics
01/06/2013 → 02/06/2013
San Diego - California, United States
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Inorganic Chemistry (Journal)
Period: May 2013
Ngo Van Nong (Reviewer)
Department of Energy Conversion and Storage
Electrofunctional materials
Description
Inorganic Chemistry
Related journal
Inorganic Chemistry
0020-1669
Central database
Activity: Research › Peer review of manuscripts

Sustainable fuels from renewable energy
Period: 22 May 2013
Mogens Bjerg Mogensen (Lecturer)
Department of Energy Conversion and Storage
Fundamental Electrochemistry
Description
Spring School: Smart energy Solutions in Urban Environment.
Related event
Spring School: Smart energy Solutions in Urban Environment
21/05/2013 → 25/05/2013
Pra Catinat, Italy
Activity: Talks and presentations › Conference presentations

Seminar Activity in Politecnico di Torino
Period: 21 May 2013
Mogens Bjerg Mogensen (Invited speaker)
Department of Energy Conversion and Storage
Fundamental Electrochemistry
Description
Title of presentation: Sustainable fuels from renewable energy.
Seminar Activity in Politecnico di Torino.
Related event
Seminar Activity in Politecnico di Torino
21/05/2013 → …
Torino, Italy
Activity: Talks and presentations › Conference presentations
9th International Symposium on Hysteresis Modelling and Micromagnetics
Period: 13 May 2013 → 15 May 2013
Lars von Moos (Speaker)
Department of Energy Conversion and Storage
Electrofunctional materials

Related event

9th International Symposium on Hysteresis Modelling and Micromagnetics
13/05/2013 → 15/05/2013
Taormina, Italy
Activity: Talks and presentations › Conference presentations

Journal of Alloys and Compounds (Journal)
Period: Apr 2013
Ngo Van Nong (Reviewer)
Department of Energy Conversion and Storage
Electrofunctional materials

Description
Journal of Alloys and Compounds

Related journal

Journal of Alloys and Compounds
0925-8388
Central database
Activity: Research › Peer review of manuscripts

Materials Research Bulletin (Journal)
Period: Apr 2013
Ngo Van Nong (Reviewer)
Department of Energy Conversion and Storage
Electrofunctional materials

Description
Materials Research Bulletin

Related journal

Materials Research Bulletin
0025-5408
BFI (2018): BFI-level 1, Scopus rating (2017): CiteScore 2.74 SJR 0.746 SNIP 0.866, ISI indexed (2013): ISI indexed yes, Web of Science (2018): Indexed yes
Central database
Activity: Research › Peer review of manuscripts

International Energy Agency
Period: 21 Apr 2013 → 25 Apr 2013
Didier Blanchard (Speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Description
NH3 Storage in Mixed Salt – MH-Air Cell

Related event

International Energy Agency: Kickoff Meeting of Task 32 "Hydrogen-based energy storage"
21/04/2013 → 25/04/2013
Heraklion - Crete, Greece
Activity: Talks and presentations › Conference presentations

The 5th Fundamentals and Developments of Fuel Cells Conference 2013
Period: 17 Apr 2013
Mogens Bjerg Mogensen (Invited speaker)
Department of Energy Conversion and Storage
Fundamental Electrochemistry

Description
Operation temperature, materials and reversibility of fuel cells - electrolyser cells.

Related event

The 5th Fundamentals and Developments of Fuel Cells Conference 2013
16/04/2013 → 18/04/2013
Karlsruhe, Germany
Activity: Talks and presentations › Conference presentations

Identifying Ways to Improve the Efficiency of Magnetocaloric Devices
Period: 15 Apr 2013 → 19 Apr 2013
Christian Bahl (Organizer)
Department of Energy Conversion and Storage
Electrofunctional materials

Description
Joint Workshop (DTU and Federal University of Santa Catarina, Florianopolis, Brazil)
"Identifying Ways to Improve the Efficiency of Magnetocaloric Devices"
Funded by Danish Agency for Science, Technology and Innovation and to the CNPq, Brazil

Related event

Identifying Ways to Improve the Efficiency of Magnetocaloric Devices
15/04/2013 → 19/04/2013
Florianopolis, Brazil
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Identifying Ways to Increase the Efficiency of Magnetocaloric Devices
Period: 15 Apr 2013 → 19 Apr 2013
Lars von Moos (Speaker)
Risø National Laboratory for Sustainable Energy
Department of Energy Conversion and Storage
Electrofunctional materials

Description
Identifying ways to increase the efficiency of magnetocaloric devices

Related event

Identifying Ways to Increase the Efficiency of Magnetocaloric Devices
15/04/2013 → 19/04/2013
Florianopolis, Brazil
Activity: Talks and presentations › Conference presentations

Using biofuels for SOFC
Period: 13 Apr 2013
Anke Hagen (Invited speaker)
Department of Energy Conversion and Storage
Applied Electrochemistry

Related event

2nd International Symposium on Solid Oxide Fuel Cells for Next Generation Power Plants: SOFCs and Renewable Energy
19/04/2013 → …
London, United Kingdom
Activity: Talks and presentations › Conference presentations

Electrolysis and CO2-Recycling for Production of Green Fuels
Period: 9 Apr 2013
Søren Linderoth (Lecturer)
Department of Energy Conversion and Storage

Description
Indlæg ved Conference

Related event

Electrolysis and CO2-Recycling for Production of Green Fuels
09/04/2013 → 11/04/2013
Roskilde, Denmark
Activity: Talks and presentations › Conference presentations

Workshop on Electrolysis and CO2-Recycling for Production of Green Fuels
Period: 9 Apr 2013 → 11 Apr 2013
Mogens Bjerg Mogensen (Organizer)
Department of Energy Conversion and Storage
Fundamental Electrochemistry

Description
Co-chairman together with Prof. Klaus S. Lackner, Columbia University, NY, USA.

Co-chair and organizer of the workshop: Electrolysis and CO2-Recycling for Production of Green Fuels
DTU Risø Campus, Roskilde, Denmark - April 9 – 11, 2013

Related event

Workshop on Electrolysis and CO2-Recycling for Production of Green Fuels
09/04/2013 → 11/04/2013
Roskilde, Denmark
Activity: Attending an event › Participating in or organising a conference

Workshop on Electrolysis and CO2-Recycling for Production of Green Fuels
Period: 9 Apr 2013
Mogens Bjerg Mogensen (Speaker)
Fundamental Electrochemistry
Department of Energy Conversion and Storage

Description
Perspectives in Electrolysis and CO2-Recycling.
Introductory talk "Perspectives in Electrolysis and CO2-Recycling" to the Workshop on Electrolysis and CO2-Recycling for Production of Green Fuels.

Related event

Workshop on Electrolysis and CO2-Recycling for Production of Green Fuels
09/04/2013 → 11/04/2013
Roskilde, Denmark
Activity: Talks and presentations › Conference presentations

Computational screening of mixed metal halide ammines
Period: 8 Apr 2013
Peter Bjerre Jensen (Lecturer)
Department of Energy Conversion and Storage
Theoretical Atomic-scale Physics
Atomic scale modelling and materials

Related event

245th ACS National Meeting & Exposition
07/04/2013 → 11/04/2013
New Orleans, LA, United States
Activity: Talks and presentations › Conference presentations

Collaboration between DTU and Topsoe Fuel Call
Period: 20 Mar 2013
Søren Linderoth (Lecturer)
Department of Energy Conversion and Storage

Related event

Open Inspiration : Denmark - the green test land of oppotunity
20/03/2013 → …
Kgs. Lyngby, Denmark
Activity: Talks and presentations › Conference presentations

Renewable Energy Technologies: Possible Collaboration Between Denmark and Japan
Period: 9 Mar 2013
Søren Linderoth (Speaker)
Department of Energy Conversion and Storage

Related event

Pugwash: Remembering Fukushima
09/03/2013 → …
København, Denmark
Activity: Talks and presentations › Conference presentations

Electronic Materials Letters (Journal)
Period: Feb 2013
Ngo Van Nong (Reviewer)
Department of Energy Conversion and Storage
Electrofunctional materials

Related journal

Electronic Materials Letters
1738-8090
Scopus rating (2017): CiteScore 2.15 SJR 0.704 SNIP 1.031, Web of Science (2018): Indexed yes
Local database
Activity: Research › Peer review of manuscripts

Department of Energy Conversion and Storage
Period: 26 Feb 2013
Søren Linderoth (Lecturer)
Department of Energy Conversion and Storage

Related event

Korean-Danish Green Technology Workshop
25/02/2013 → 27/02/2013
Seoul, Korea, Republic of
Activity: Talks and presentations › Conference presentations

3rd Magnetism National Conference
Period: 20 Feb 2013 → 22 Feb 2013
Lars von Moos (Participant)
Department of Energy Conversion and Storage
Electrofunctional materials

Description
Participation in conference
Documents:
Poster_Magnet2013

Related event

3rd Magnetism National Conference
20/02/2013 → 22/02/2013
Naples, Italy
Activity: Attending an event › Participating in or organising a conference

Nanostructured materials for solid-state hydrogen storage – WG4: Computational modeling
Period: 25 Jan 2013
Tejs Vegge (Invited speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related event

COST MP1103 Network Meeting
25/01/2013 → …
Stoos, Switzerland
Activity: Talks and presentations › Conference presentations

The Importance of Nano Science in Energy Technologies
Period: 22 Jan 2013 → 23 Jan 2013
Søren Linderoth (Lecturer)
Department of Energy Conversion and Storage

Related event

Orchestrated NanoKnowledge: Energy, Surface and Nanomedicine
22/01/2013 → 23/01/2013
Copenhagen, Denmark
Activity: Talks and presentations › Conference presentations
PALSfit; website: palsfit.dk: A computer code for analysing positron annihilation lifetime spectra.
Period: 1 Jan 2013 → …
Morten Mostgaard Eldrup (Participant)

Department of Energy Conversion and Storage
Atomic scale modelling and materials

**Description**
PALSfit is a computer program for analysing spectra that are measured by positron annihilation lifetime spectroscopy (PALS). PALSfit is based on the well tested PATFIT program, which has been used extensively by the positron annihilation community. Taking advantage of the windows interface, a number of user friendly facilities have been incorporated, in particular graphics displays.

Links:
http://palsfit.dk

**Related external organisation**
Morten Eldrup, Jens V. Olsen, Peter Kirkegaard and Niels Jørgen Pedersen
Denmark
Activity: Other

Advanced Materials (Journal)
Period: 2012
Ngo Van Nong (Reviewer)
Department of Energy Conversion and Storage
Electrofunctional materials

**Related journal**
Advanced Materials

American Physical Society (External organisation)
Period: 2012 → …
Duc-The Ngo (Participant)

Department of Energy Conversion and Storage
Imaging and Structural Analysis
Department of Micro- and Nanotechnology
Molecular Windows
Degree of recognition: International

**Related external organisation**
American Physical Society
United States
Activity: Membership › Membership of research networks or expert groups

Applied Physics Letters (Journal)
Period: 2012 → 2014
Duc-The Ngo (Reviewer)
Department of Energy Conversion and Storage
Imaging and Structural Analysis
Department of Micro- and Nanotechnology

Molecular Windows

Description
I work quite regularly as a reviewer for Applied Physics Letters in the topic of nanomagnetism and spintronics from 2012

Related journal
Applied Physics Letters
0003-6951
Central database
Activity: Research › Peer review of manuscripts

PhD thesis Alfred Samson: Censor
Period: 2012
Anke Hagen (External examiner)
Department of Energy Conversion and Storage

Applied Electrochemistry
Activity: Examinations and supervision › External examination

Self assembled dimers of metallic nano-particles for enhanced light harvesting in organic solar cells
Period: 2012 → …
Francesco Pastorelli (Speaker)
Department of Energy Conversion and Storage

Functional organic materials

Related event
5th Mediterranean Conference on NanoPhotonics
05/11/2012 → 06/11/2012
Barcelona, Spain
Activity: Talks and presentations › Conference presentations

Self assembled dimers of metallic nano-particles for enhanced light harvesting in organic solar cells
Period: 2012 → …
Francesco Pastorelli (Speaker)
Department of Energy Conversion and Storage

Functional organic materials

Related event
Conferencia Española de Nanofotonica 2012
01/10/2012 → 04/10/2012
Sevilla, Spain
Activity: Talks and presentations › Conference presentations

Strategy Group (External organisation)
Period: 2012 → 2015
Anke Hagen (Participant)
Department of Energy Conversion and Storage

Applied Electrochemistry

Description
Under Partnership for Hydrogen and Fuel Cells
Related external organisation

Strategy Group
Activity: Membership › Membership of committees, commissions, boards, councils, associations, organisations, or similar

Ergebnisse aus Langzeittests von Einzelzellen
Period: Dec 2012
Anke Hagen (Lecturer)
Department of Energy Conversion and Storage
Applied Electrochemistry

Related event

2nd SOFC Workshop „Reproduzierbares Testen von SOFC Einzelzellen - aktuelle Entwicklungen in Standardisierung und Charakterisierung”
17/12/2012 → 18/12/2012
Barleben, Germany
Activity: Talks and presentations › Conference presentations

Design, Modeling and Optimization of Thermoelectrical Power Generation Devices
Period: 10 Dec 2012
Nini Pryds (External examiner)
Department of Energy Conversion and Storage
Electrofunctional materials

Description
PHD Examiner
Activity: Examinations and supervision › External examination

Nordic Conference on Ceramic and Glass Technology
Period: 6 Dec 2012 → 7 Dec 2012
Francesca Teocoli (Participant)
Department of Energy Conversion and Storage
Ceramic Engineering & Science

Description
Shape distortion and thermo-mechanical properties of SOFC components from green tape to sintered body
Documents:
Abstract_Nordic_Conference_Teocoli.pdf

Related event

Nordic Conference on Ceramic and Glass Technology
06/12/2012 → 07/12/2012
Roskilde, Denmark
Activity: Attending an event › Participating in or organising a conference

Computational Screening of Mixed Metal Halide Ammines
Period: 4 Dec 2012
Peter Bjerre Jensen (Lecturer)
Department of Energy Conversion and Storage
Atomic scale modelling and materials
Department of Physics

Related event
1st European Early Stage Researchers' Conference on Hydrogen Storage
03/12/2012 → 05/12/2012
Belgrade, Serbia
Activity: Talks and presentations › Conference presentations

6th International Workshop on Advanced Materials Science and Nanotechnology
Period: Nov 2012
Ngo Van Nong (Keynote speaker)
Department of Energy Conversion and Storage
Electrofunctional materials
Description
Nanostructured Thermoelectric Oxide Materials and Modules for Effective Power Generation from Waste Heat

Related event
6th International Workshop on Advanced Materials Science and Nanotechnology
30/10/2012 → 02/11/2012
Ha Long City, Viet Nam
Activity: Talks and presentations › Conference presentations

Degradation of state-of-the-art SOFC in hydrogen and carbon containing fuels
Period: Nov 2012
Anke Hagen (Invited speaker)
Department of Energy Conversion and Storage
Applied Electrochemistry
Related event
Workshop on Sulfur Poisoning of Solid Oxide Cells, Risø Campus
19/11/2012 → …
Risø, Denmark
Activity: Talks and presentations › Conference presentations

2012 MRS Fall Meeting & Exhibit
Nini Pryds (Organizer)
Department of Energy Conversion and Storage
Electrofunctional materials
Description
Oxide Thin Films for Renewable Energy Applications
Related event
2012 MRS Fall Meeting & Exhibit
25/11/2012 → 30/11/2012
Boston, MA, United States
Activity: Attending an event › Participating in or organising a conference

Electrolysis and biomass hand-in-hand
Period: 15 Nov 2012
Søren Linderoth (Lecturer)
Department of Energy Conversion and Storage
Management

Related event

Conference on Energy Security: Outlook & Perspectives in the Baltic Sea Region
15/11/2012 → 16/11/2012
Vilnius, Lithuania
Activity: Talks and presentations › Conference presentations

Oxides in Environment-friendly Technologies
Period: 3 Nov 2012
Nini Pryds (Invited speaker)
Electrofunctional materials
Department of Energy Conversion and Storage

Description
Invited speaker at our G-COE International Symposium, Japan
http://ncrs.cm.kyushu-u.ac.jp/ncrs2/home.html
Oxides in Environment-friendly Technologies

Related external organisation

Unknown external organisation
Activity: Talks and presentations › Conference presentations

Final SERC Technical-Scientific Meeting
Period: 1 Nov 2012
Peter Blennow Tullmar (Speaker)
Department of Energy Conversion and Storage
Ceramic Engineering & Science

Description
Presented a summary of the results obtained within SERC on new materials for solid oxide cells
New materials for solid oxide cells - nanostructured electrocatalysts by infiltration and/or exsolution

Related event

Final SERC Technical-Scientific Meeting
01/11/2012 → …
Roskilde, Denmark
Activity: Talks and presentations › Conference presentations

Ceramics International (Journal)
Period: Oct 2012 → …
Ngo Van Nong (Reviewer)
Department of Energy Conversion and Storage
Electrofunctional materials

Description
Ceramics International

Related journal

Ceramics International
0272-8842
BFI (2018): BFI-level 1, Scopus rating (2017): CiteScore 2.85 SJR 0.784 SNIP 1.167, ISI indexed (2013): ISI indexed yes,
Web of Science (2018): Indexed yes
6th International Workshop on Advanced Materials Science and Nanotechnology
Thanh Hung Le (Speaker)
Department of Energy Conversion and Storage
Electrofunctional materials

Description
Geometry optimization on high temperature oxide thermoelectric power generation

Oral presentation

Related event

6th International Workshop on Advanced Materials Science and Nanotechnology
30/10/2012 → 02/11/2012
Ha Long City, Viet Nam
Activity: Talks and presentations › Conference presentations

6th International Workshop on Advanced Materials Science and Nanotechnology
Ngo Van Nong (Speaker)
Department of Energy Conversion and Storage
Electrofunctional materials

Description
High-Temperature segmented thermoelectric oxide module using p-type Ca$_3$Co$_4$O$_9$ and n-type ZnAlO/CaMn$_{0.95}$Nb$_{0.05}$O$_3$ legs

Documents:
Abstract

Related event

6th International Workshop on Advanced Materials Science and Nanotechnology
30/10/2012 → 02/11/2012
Ha Long City, Viet Nam
Activity: Talks and presentations › Conference presentations

6th International Workshop on Advanced Materials Science and Nanotechnology
Ngo Van Nong (Speaker)
Department of Energy Conversion and Storage
Electrofunctional materials

Description
THE INFLUENCE OF BORON ADDITION ON STRUCTURAL, MAGNETIC AND THERMOELECTRIC PROPERTIES OF Ni2Mn1.52Sb0.48Bx

Documents:
Abstract

Related event

6th International Workshop on Advanced Materials Science and Nanotechnology
30/10/2012 → 02/11/2012
Ha Long City, Viet Nam
Activity: Talks and presentations › Conference presentations
6th International Workshop on Advanced Materials Science and Nanotechnology


Ngo Van Nong (Invited speaker)

Department of Energy Conversion and Storage

Electrofunctional materials

Description

Documents:
Abstract

Related event

6th International Workshop on Advanced Materials Science and Nanotechnology
30/10/2012 → 02/11/2012
Ha Long City, Viet Nam
Activity: Talks and presentations › Conference presentations

Brændselsceller og brint

Period: 24 Oct 2012

Søren Linderoth (Lecturer)

Department of Energy Conversion and Storage

Description

Undervisning ved Folkeuniversitetet

Foredragsholder ved Folkeuniversitetet - Herning

Related external organisation

Folkeuniversitetet i Herning
Herning, Denmark
Activity: Talks and presentations › Guest lectures, external teaching and course activities at other universities

Mixed Rare Earth-Fe-B sintered magnets

Period: 24 Oct 2012

Christian Bahl (Lecturer)

Department of Energy Conversion and Storage

Electrofunctional materials

Related event

Applied Magnetic Materials
24/10/2013 → 25/10/2013

Pori, Finland
Activity: Talks and presentations › Conference presentations

International Symposium on Metal-Hydrogen Systems - Fundamentals and Applications -


Didier Blanchard (Participant)

Department of Energy Conversion and Storage

Atomic scale modelling and materials

Description

Two Posters presentations - QENS in Ca and Mg Borohydrides - Ammonia Storage in Metal Salts
Related event

**International Symposium on Metal-Hydrogen Systems - Fundamentals and Applications -**
21/10/2012 → 26/10/2012
Kyoto, Japan
Activity: Attending an event › Participating in or organising a conference

**Metal Borohydrides for Hydrogen Storage: A Review**
Period: 21 Oct 2012
Didier Blanchard (Invited speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related event

**BiT's 2nd New Energy Forum - 2012: Hydrogen energy**
19/10/2012 → 21/10/2012
Guangzhou, China
Activity: Talks and presentations › Conference presentations

**Department of Energy Conversion and Storage**
Period: 17 Oct 2012
Søren Linderoth (Lecturer)
Department of Energy Conversion and Storage

**Description**
Oplæg ved SK Innovation Global Technology, Daejeon, Korea

**Related external organisation**

**Unknown external organisation**
Activity: Talks and presentations › Conference presentations

**Solid oxide electrochemical cells – energy converters, gas separators, gas sensors**
Period: 14 Oct 2012
Mogens Bjerg Mogensen (Lecturer)
Fundamental Electrochemistry
Department of Energy Conversion and Storage
Department of Physics

Related event

**iNANO Autumn School 2012**
12/10/2012 → 15/10/2012
Grenå, Denmark
Activity: Talks and presentations › Conference presentations

**SERC Workshop**
Period: 8 Oct 2012
Søren Linderoth (Speaker)
Department of Energy Conversion and Storage

Related event

**SERC Workshop**
08/10/2012 → ...
København, Denmark
Activity: Talks and presentations › Conference presentations
Computational investigations of the electronic transport in lithium-air battery materials
Tejs Vegge (Speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related event
Pacific Rim Meeting on Electrochemical and Solid-State Science: 222nd Meeting of ECS — The Electrochemical Society and 2012 Fall Meeting of The Electrochemical Society of Japan
07/10/2012 → 12/10/2012
Honolulu, United States
Activity: Talks and presentations › Conference presentations

Istituto Nazionale di Ricerca Metrologica
Period: 1 Oct 2012 → 17 Dec 2012
Lars von Moos (Visiting researcher)
Department of Energy Conversion and Storage
Electrofunctional materials

Description
Research stay: Collaboration with research group
Activity: Visiting an external institution › Visiting another research institution

Journal of Electronic Materials (Journal)
Period: Sep 2012 → …
Ngo Van Nong (Reviewer)
Department of Energy Conversion and Storage
Electrofunctional materials

Description
Journal of Electronic Materials

Related journal
Journal of Electronic Materials
0361-5235
Central database
Activity: Research › Peer review of manuscripts

Pure and Applied Chemistry (Journal)
Period: Sep 2012 → …
Ngo Van Nong (Reviewer)
Department of Energy Conversion and Storage
Electrofunctional materials

Description
Pure and Applied Chemistry

Related journal
Pure and Applied Chemistry
0033-4545
Solid State Electrochemistry Applied to Solid Oxide Fuel and Electrolysis Cells
Period: Sep 2012
Anke Hagen (Invited speaker)
Department of Energy Conversion and Storage
Applied Electrochemistry

Related event
Electrochemistry 2012
17/09/2012 → 23/09/2012
München, Germany
Activity: Talks and presentations › Conference presentations

Alkaline Electrolysis Cells: Materials, Properties and Challenges
Period: 25 Sep 2012
Mogens Bjerg Mogensen (Lecturer)
Fundamental Electrochemistry
Department of Energy Conversion and Storage
Department of Physics

Description
Lecture at 2nd Joint European Summer School on Fuel Cells and Hydrogen Technology.

Related event
2nd Joint European Summer School on Fuel Cell and Hydrogen Technology
17/09/2012 → 28/09/2012
Heraklion, Greece
Activity: Talks and presentations › Conference presentations

History of Thermodynamics of Electrolysis
Period: 25 Sep 2012
Mogens Bjerg Mogensen (Lecturer)
Fundamental Electrochemistry
Department of Energy Conversion and Storage
Department of Physics

Description
Lecture at 2nd Joint European Summer School on Fuel Cells and Hydrogen Technology

Related event
2nd Joint European Summer School on Fuel Cell and Hydrogen Technology
17/09/2012 → 28/09/2012
Heraklion, Greece
Activity: Talks and presentations › Conference presentations

5th IIF-IIR International Conference on Magnetic Refrigeration at Room Temperature
Period: 18 Sep 2012
Christian Bahl (Speaker)
Department of Energy Conversion and Storage
Electrofunctional materials
Description
Invited speaker

Development and Experimental Results from a 1 kW Prototype AMR

Related event
5th IIF-IIR International Conference on Magnetic Refrigeration at Room Temperature
17/09/2012 → 20/09/2012
Grenoble, France
Activity: Talks and presentations » Conference presentations

5th IIF-IIR International Conference on Magnetic Refrigeration at Room Temperature
Period: 18 Sep 2012
Kurt Engelbrecht (Speaker)
Department of Energy Conversion and Storage
Electrofunctional materials

Description
Gave presentation titled "Material Properties and Modeling Characteristics for MnFePAs Materials for Application in Magnetic Refrigeration"

Related event
5th IIF-IIR International Conference on Magnetic Refrigeration at Room Temperature
17/09/2012 → 20/09/2012
Grenoble, France
Activity: Talks and presentations » Conference presentations

Development and Experimental Results from a 1kW Prototype AMR
Period: 18 Sep 2012
Christian Bahl (Invited speaker)
Electrofunctional materials
Department of Energy Conversion and Storage

Related event
5th IIF-IIR International Conference on Magnetic Refrigeration at Room Temperature
17/09/2012 → 20/09/2012
Grenoble, France
Activity: Talks and presentations » Conference presentations

5th IIF-IIR International Conference on Magnetic Refrigeration at Room Temperature
Period: 17 Sep 2012 → 20 Sep 2012
Lars von Moos (Speaker)
Department of Energy Conversion and Storage
Electrofunctional materials

Description
Talk at Thermag 5 Conference, Grenoble Italy

Related event
5th IIF-IIR International Conference on Magnetic Refrigeration at Room Temperature
17/09/2012 → 20/09/2012
Grenoble, France
Activity: Talks and presentations » Conference presentations
ESS Science Symposium  
Period: 17 Sep 2012 → 19 Sep 2012  
Didier Blanchard (Participant)  
Department of Energy Conversion and Storage  
Atomic scale modelling and materials  

Description  
Poster presentation  

Related event  
ESS Science Symposium: Neutrons for Energy - Advanced Materials for Energy Storage  
17/09/2012 → 19/09/2012  
Delft, Netherlands  
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

3rd CARISMA International Conference on Medium and High Temperature Proton Exchange Membrane Fuel Cells  
Period: 3 Sep 2012  
Søren Linderoth (Speaker)  
Department of Energy Conversion and Storage  

Related event  
3rd CARISMA International Conference on Medium and High Temperature Proton Exchange Membrane Fuel Cells  
03/09/2012 → 05/09/2012  
Copenhagen, Denmark  
Activity: Talks and presentations › Conference presentations

Årsmøde 2013 i Dansk Batteriselskab  
Period: 1 Sep 2012 → 1 Mar 2013  
Jonathan Højberg (Organizer)  
Department of Energy Conversion and Storage  
Atomic scale modelling and materials  

Description  
Medstifter af Dansk Batteriselskab og medarrangør af arrangementet  
Links:  
http://batteriselskab.dk/founding_meeting  

Related event  
Årsmøde 2013 i Dansk Batteriselskab  
01/03/2013 → …  
Roskilde, Denmark  
Activity: Attending an event › Participating in or organising a conference

SUNCAT Center for Interface Science and Catalysis  
Period: 1 Sep 2012 → 30 Nov 2012  
Tejs Vegge (Visiting researcher)  
Department of Energy Conversion and Storage  
Atomic scale modelling and materials  

Description  
Visiting Professor : SUNCAT at SLAC National Accelerator and Department of Chemical Engineering, Stanford University  
Activity: Visiting an external institution › Visiting another research institution
Vacuum (Journal)
Period: Aug 2012 → …
Ngo Van Nong (Reviewer)
Department of Energy Conversion and Storage
Electrofunctional materials

Description
Vacuum

Related journal
Vacuum
0042-207X
Central database
Activity: Communication › Peer review of manuscripts

Computational Design of Materials for Energy Storage
Period: 11 Aug 2012 → 17 Aug 2012
Tejs Vegge (Invited speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related event
CAMD Summer School in Electronic Structure Theory and Materials Design
11/08/2012 → 17/08/2012
Lyngby, Denmark
Activity: Talks and presentations › Conference presentations

Reversible Lithium-Air Batteries
Period: 10 Aug 2012
Tejs Vegge (Lecturer)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related event
1st International ReLiable Workshop
10/08/2012 → 10/08/2012
Copenhagen, Denmark
Activity: Talks and presentations › Conference presentations

In situ XRPD studies of Li intercalation in graphite in working Li-ion batteries: Session: MS13 - Energy related materials
Rune E. Johnsen (Lecturer)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related event
27th Meeting of the European Crystallographic Association
06/08/2012 → 11/08/2012
Bergen, Norway
Activity: Talks and presentations › Conference presentations
A Materials Science Perspective on the Mechanics of Sintering
Period: 20 Jul 2012
Rasmus Bjørk (Lecturer)
Department of Energy Conversion and Storage
Electrofunctional materials

Description
Presented at: CEA Cadarache, France

Related external organisation
Unknown external organisation
Activity: Talks and presentations › Conference presentations

12th International Conference on Inorganic Membrane
Period: 13 Jul 2012
Kurt Engelbrecht (Speaker)
Department of Energy Conversion and Storage
Electrofunctional materials

Description
Mechanical analysis of tubular oxygen membranes for robust membrane modules

Related event
12th International Conference on Inorganic Membrane
09/07/2012 → 13/09/2012
Eschede, Netherlands
Activity: Talks and presentations › Conference presentations

31st International & 10th European Conference on Thermoelectrics
Period: 11 Jul 2012
Li Han (Speaker)
Department of Energy Conversion and Storage

Description
Presentation of 'The Influence of Spark Plasma Sintering Temperature on the Thermoelectric Properties of Al, Ga dually-doped ZnO'

Related event
31st International & 10th European Conference on Thermoelectrics
09/07/2012 → 12/07/2012
Aalborg, Denmark
Activity: Talks and presentations › Conference presentations

31st International & 10th European Conference on Thermoelectrics
Period: 9 Jul 2012
Thanh Hung Le (Participant)
Department of Energy Conversion and Storage
Electrofunctional materials

Description
Oral presentation

Related event
31st International & 10th European Conference on Thermoelectrics
09/07/2012 → 12/07/2012
Aalborg, Denmark
Activity: Attending an event › Participating in or organising a conference

**Plasma Sheath Lenses - Principles and applications**
Period: 2 Jul 2012 → 6 Jul 2012
Eugen Stamate (Invited speaker)
Department of Energy Conversion and Storage
Electrofunctional materials

**Description**
award invited lecture

**Related event**

*39th European Physical Society Conference on Plasma Physics and 16th International Congress on Plasma Physics*
02/07/2012 → 06/07/2012
Stockholm, Sweden
Activity: Talks and presentations › Conference presentations

European Fuel Cell Forum 2012
Period: 30 Jun 2012 → 3 Jul 2012
Anne Hauch (Participant)
Department of Energy Conversion and Storage

**Description**
Deltager samt poster bidrag

**Multilayer Tape Cast SOFC - Effect of Anode Sintering Temperature**

**Documents:**
EFCF_poster_cbir_2012-06-22_hauc_edit_FINAL

**Related event**

*European Fuel Cell Forum 2012*
27/06/2012 → 29/06/2012
Luzern, Switzerland
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

European Fuel Cell Forum 2012
Peter Blennow Tullmar (Speaker)
Department of Energy Conversion and Storage
Ceramic Engineering & Science

**Description**
Poster presentation at the conference: Infiltrated SrTiO$_3$:FeCr-based anodes for metal-supported SOFC

**Related event**

*European Fuel Cell Forum 2012*
27/06/2012 → 29/06/2012
Luzern, Switzerland
Activity: Talks and presentations › Conference presentations

**Rotational and translational diffusion in materials for energy storage from QENS and DFT calculations**
Tejs Vegge (Invited speaker)
Department of Energy Conversion and Storage

Atomic scale modelling and materials

Related event

2nd Annual Niels Bohr International Academy Workshop on Neutron Science: Bridging Elastic and Inelastic Scattering by means of Computational Studies and Analysis
25/06/2012 → 29/06/2012
Copenhagen, Denmark
Activity: Talks and presentations › Conference presentations

Computational techniques for efficient design of nanoparticles and complex materials for energy storage
Period: 13 Jun 2012 → 18 Jun 2012
Tejs Vegge (Lecturer)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Related event

International Conference on Materials for Hydrogen Storage – Future and Perspectives
13/06/2012 → 18/06/2012
Hurtigruten, Norway
Activity: Talks and presentations › Conference presentations

Development of SOEC Cells and Stacks: Highlights, Challenges and future Perspectives
Period: 5 Jun 2012
Wolff-Ragnar Kiebach (Keynote speaker)
Department of Energy Conversion and Storage
Mixed Conductors

Related event

World Hydrogen Energy Conference 2012
03/06/2012 → 07/06/2012
Toronto, Canada
Activity: Talks and presentations › Conference presentations

Department of Energy Conversion and Storage
Period: May 2012
Søren Linderoth (Lecturer)
Department of Energy Conversion and Storage

Description
Mundtligt oplæg ved besøg hos Samsung Advanced Institute of Technology (SAIT, Suwan, Korea

Related external organisation

Unknown external organisation
Activity: Talks and presentations › Conference presentations

SOFC Durability under Realistic Operation
Period: May 2012
Anke Hagen (Lecturer)
Department of Energy Conversion and Storage
Applied Electrochemistry
Related event

10th International Symposium on Ceramic Materials and Components for Energy and Environmental Applications
07/05/2012 → 12/05/2012
Dresden, Germany
Activity: Talks and presentations › Conference presentations

SYMPOSIUM Water Electrolysis and Hydrogen as Part of the Future Renewable Energy System
Period: May 2012
Anke Hagen (Organizer)
Department of Energy Conversion and Storage
Applied Electrochemistry

Related event

SYMPOSIUM Water Electrolysis and Hydrogen as Part of the Future Renewable Energy System
10/05/2012 → 11/05/2012
Copenhagen, Denmark
Activity: Attending an event › Participating in or organising a conference

Werkstofffragen der Hochtemperatur-Brennstoffzelle (SOFC): Risø/Topsoe SOFC Aktivitäten
Period: May 2012
Anke Hagen (Lecturer)
Department of Energy Conversion and Storage
Applied Electrochemistry

Description
Contribution to course

Related external organisation

Unknown external organisation
Activity: Talks and presentations › Conference presentations

42nd Danish Crystallographic Meeting and 5th DanScatt Meeting
Period: 31 May 2012 → 1 Jun 2012
Rune E. Johnsen (Participant)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Description
Poster presentation: "In situ synchrotron X-ray diffraction studies of large and small lithium batteries (from 10Ah to 0.1 mAh)"

Related event

42nd Danish Crystallographic Meeting and 5th DanScatt Meeting
31/05/2012 → 01/06/2012
Odense, Denmark
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

European Materials Research Society 2012
Period: 30 May 2012
Li Han (Participant)
Department of Energy Conversion and Storage

Description
Presentation of 'the influence of including α- or γ-Al2O3 phases in Al-doped ZnO on the Thermoelectric Properties'
Related event

European Materials Research Society 2012: Symposium D, Unconventional Thermoelectrics: From new materials to energy conversion devices
27/05/2012 → 31/05/2012
Strasbourg, France
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

FIB Damage and Polishing in 3DEBSD of ceramic materials
Period: 24 May 2012
Jacob R. Bowen (Speaker)
Department of Energy Conversion and Storage
Imaging and Structural Analysis

Description
Oxford Instruments EBSD user group meeting
Talk Title: FIB Damage and Polishing in 3DEBSD of ceramic materials
Documents:
FIB Damaging and Polishing in 3DEBSD of ceramic materials

Related event

Oxford Instruments EBSD Symposium
23/05/2012 → 24/05/2012
Weisbaden, Germany
Activity: Talks and presentations › Conference presentations

European Materials Research Society 2012
Period: 14 May 2012
Thanh Hung Le (Participant)
Department of Energy Conversion and Storage
Electrofunctional materials

Description
Poster presentation

Related event

European Materials Research Society 2012: Symposium D, Unconventional Thermoelectrics: From new materials to energy conversion devices
27/05/2012 → 31/05/2012
Strasbourg, France
Activity: Attending an event › Participating in or organising a conference

SYMPOSIUM Water Electrolysis and Hydrogen as Part of the Future Renewable Energy System
Period: 10 May 2012 → 11 May 2012
Jacob R. Bowen (Participant)
Department of Energy Conversion and Storage
Imaging and Structural Analysis

Description
Selected hydrogen production activities at the Institut of Technical Thermodynamics of DLR focused on the electrodes and stack design

The Institute of Technical Thermodynamics started developing various kinds of electrolyzers for a large range of applications approx. in 1985. The main topics are the development of stabilized electrodes for applications with drastical load changes and high durability as well as the understanding of mechanisms and degradation effects.
Documents:
Selected hydrogen production activities at the Institute of Technical Thermodynamics of DLR focused on the electrodes and stack design

Links:
http://indico.conferences.dtu.dk/conferenceDisplay.py?confId=102 (Symposium website)

Related event

**SYMPOSIUM Water Electrolysis and Hydrogen as Part of the Future Renewable Energy System**
10/05/2012 → 11/05/2012
Copenhagen, Denmark
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

**Metal-supported Solid Oxide Fuel Cells: Next generation SOFCs?: Invited talk**
Period: 30 Mar 2012
Peter Blennow Tullmar (Speaker)
Department of Energy Conversion and Storage
Ceramic Engineering & Science

Related event

**Lund Fuel Cell Research Network meeting**
30/03/2012 → 30/03/2012
Lund, Sweden
Activity: Talks and presentations › Conference presentations

**4th User Meeting at the FRM II**
Period: 23 Mar 2012
Didier Blanchard (Participant)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

**Description**
Poster Presentation - Hindered rotational energy barriers of BH4 - tetrahedra in beta-Mg(BH4)2 from quasieelastic neutron scattering and DFT calculations

**User Meeting at FRM II - Munich**

Related event

**4th User Meeting at the FRM II**
23/03/2012 → ...
Munich, Germany
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

**Reconstructions at complex oxide Interfaces**
Period: 23 Mar 2012
Nini Pryds (External examiner)
Department of Energy Conversion and Storage
Electrofunctional materials

**Description**
Members of the examining committee.
Activity: Examinations and supervision › External examination

**Tohoku University**
Dadi Þorsteinn Sveinbjörnsson (Visiting researcher)
Department of Energy Conversion and Storage

Description
External research stay
Activity: Visiting an external institution › Visiting another research institution

Nanostructured materials for solid-state hydrogen storage - MPNS COST Action MP1103
Peter Bjerre Jensen (Participant)
Department of Energy Conversion and Storage
Atomic scale modelling and materials
Department of Physics

Related event
Nanostructured materials for solid-state hydrogen storage - MPNS COST Action MP1103
13/02/2012 → 15/02/2012
Roma, Italy
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Nanostructured materials for solid-state hydrogen storage - MPNS COST Action MP1103
Didier Blanchard (Speaker)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

Description
Presentation of the research activities on Solid-State Hydrogen Storage at DTU -Energy Conversion and Storage.
Oral presentation

Related event
Nanostructured materials for solid-state hydrogen storage - MPNS COST Action MP1103
13/02/2012 → 15/02/2012
Roma, Italy
Activity: Talks and presentations › Conference presentations

Thermoelectric Oxide Materials for Heat Recovery
Period: 9 Feb 2012
Nini Pryds (Lecturer)
Department of Energy Conversion and Storage
Electrofunctional materials

Related external organisation
Unknown external organisation
Activity: Talks and presentations › Conference presentations

Durability of Solid Oxide Fuel Cells and Solid Oxide Electrolysis Cells: Status and Challenges
Period: Jan 2012
Anke Hagen (Invited speaker)
Department of Energy Conversion and Storage
Applied Electrochemistry
Related event

**Meeting of the SOFC Society of Japan**

*20/01/2012 → …*
Tokyo, Japan
Activity: Talks and presentations › Conference presentations

**European Fuel Cell Forum (External organisation)**

*Period: Jan 2012 → Jun 2012*
Anke Hagen (Participant)
Department of Energy Conversion and Storage
Applied Electrochemistry

**Description**
Member of Scientific Committee
Degree of recognition: International

**Related external organisation**

**European Fuel Cell Forum**
Obgardiha, CH-6043, Luzern-Adligenswil, Switzerland
Activity: Membership › Membership of committees, commissions, boards, councils, associations, organisations, or similar

**Ph.D. defense Rahimullah Sarban: “Active control using DEAP transducers”**

*Period: 30 Jan 2012*
Peter Sommer-Larsen (External examiner)
Department of Energy Conversion and Storage

**Description**
Censor: Ph.D. defense Rahimullah Sarban: “Active control using DEAP transducers”
Activity: Examinations and supervision › External examination

**Studienævn DTU Energii (External organisation)**

*Period: 1 Jan 2012 → 31 Dec 2020*
Anne Hauch (Chairman)
Department of Energy Conversion and Storage
Applied Electrochemistry

**Description**
Formand for DTU Energis studienævn
Body type: Institutstudienævn

**Related external organisation**

**Studienævn DTU Energii**
Activity: Membership › Membership of committees, commissions, boards, councils, associations, organisations, or similar

**Annual Meeting International Energy Agency (IEA) Annex 24 (Solid Oxide Fuel Cells) (External organisation)**

*Period: 2011 → 2015*
Anke Hagen (Participant)
Department of Energy Conversion and Storage
Applied Electrochemistry
Degree of recognition: International

**Related external organisation**

**Annual Meeting International Energy Agency (IEA) Annex 24 (Solid Oxide Fuel Cells)**
PhD Thesis Alfred Samson
Period: 2011 → Apr 2012
Anke Hagen (Internal examiner)
Department of Energy Conversion and Storage
Applied Electrochemistry
Activity: Examinations and supervision › Internal examination

Thin Solid Films (Journal)
Period: 2011 → 2014
Duc-The Ngo (Reviewer)
Department of Energy Conversion and Storage
Imaging and Structural Analysis
Department of Micro- and Nanotechnology
Molecular Windows
Description
I have regularly worked as referee for the journal of Thin Solid Films since 2011

2nd International Workshop on Degradation Issues of Fuel Cells
Period: Sep 2011
Anke Hagen (Participant)
Department of Energy Conversion and Storage
Applied Electrochemistry

2nd Workshop on Degradation Issues
05/09/2011 → 09/09/2011
Thessaloniki, Greece
Activity: Talks and presentations › Conference presentations

Assessing durability of SOFC stacks
Period: Sep 2011
Anke Hagen (Lecturer)
Department of Energy Conversion and Storage
Applied Electrochemistry

Related event
2nd Workshop on Degradation Issues
Thessaloniki, Greece
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.
Journal of Alloys and Compounds (Journal)
Period: Sep 2011 → …
Ngo Van Nong (Reviewer)
Department of Energy Conversion and Storage
Electrofunctional materials

Description
Journal of alloys and compounds

Related journal
Journal of Alloys and Compounds
0925-8388
Central database
Activity: Research › Journal editor

Proton conductivity – mechanisms and materials
Qingfeng Li (Lecturer)
Department of Energy Conversion and Storage
Proton conductors

Related event
PROCON Summer school
16/08/2011 → 17/08/2011
Changchun, China
Activity: Talks and presentations › Guest lectures, external teaching and course activities at other universities

Troisième Cycle Seminar in Villars
Li Han (Participant)
Department of Energy Conversion and Storage

Related event
Troisième Cycle Seminar in Villars: Synthesis and Function of Thermoelectric Materials
14/08/2011 → 18/08/2011
Villars-sur-Ollon, Switzerland
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Troisième Cycle Seminar in Villars
Thanh Hung Le (Participant)
Department of Energy Conversion and Storage
Electrofunctional materials

Description
It is a summer school for PhD student.

Workshop on Synthesis and Function of Thermoelectric Materials

Related event
Troisième Cycle Seminar in Villars: Synthesis and Function of Thermoelectric Materials
14/08/2011 → 18/08/2011
Villars-sur-Ollon, Switzerland
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

**Durability and degradation of SOFCs – Where are we?**
Period: May 2011
Anke Hagen (Lecturer)
Department of Energy Conversion and Storage
Applied Electrochemistry

**Related event**

**Annual Meeting International Energy Agency (IEA) Annex 24 (Solid Oxide Fuel Cells)**
09/05/2011 → …
Montreal, Canada
Activity: Talks and presentations › Conference presentations

---

**University of New South Wales**
Period: 1 Mar 2011 → 31 May 2011
Jacob R. Bowen (Visiting researcher)
Fuel Cells and Solid State Chemistry Division
Microstructures and Interfaces
Department of Energy Conversion and Storage
Imaging and Structural Analysis

**Description**
Visiting Fellow
School of Materials Science and Engineering and the Electron Microscope Unit, UNSW
Links:
http://www.materials.unsw.edu.au/ (School of Materials Science and Engineering website)
Activity: Visiting an external institution › Visiting another research institution

---

**5th International Symposium Hydrogen & Energy**
Period: 23 Jan 2011 → 28 Jan 2011
Didier Blanchard (Participant)
Department of Energy Conversion and Storage
Atomic scale modelling and materials

**Description**
Oral Presentation: Hydrogen Rotational and Diffusional dynamics in calcium borohydride from Quasielastic Neutron Scattering and DFT.

**Related event**

**5th International Symposium Hydrogen & Energy: Empa**
23/01/2011 → 28/01/2011
Stoos, Switzerland
Activity: Attending an event › Participating in or organising a conference

---

**European Association for Storage of Energy - EASE (External organisation)**
Period: 1 Jan 2011 → 31 Dec 2017
Allan Schreder Pedersen (Participant)
Department of Energy Conversion and Storage
Centre for IT-Intelligent Energy Systems in Cities
Description
Collaboration on information and lobbying about energy storage technologies

Body type: Industry dominated private
Degree of recognition: International

Related external organisation

European Association for Storage of Energy - EASE
Activity: Membership › Board duties in companies, associations, or public organisations

European Energy Research Alliance, Joint Programme on Energy Storage (External organisation)
Period: 1 Jan 2011 → 1 Jan 2018
Allan Schrøder Pedersen (Participant)
Department of Energy Conversion and Storage
Centre for IT-Intelligent Energy Systems in Cities

Description
Steering Committee
Degree of recognition: International

Related external organisation

European Energy Research Alliance, Joint Programme on Energy Storage
Activity: Membership › Membership of committees, commissions, boards, councils, associations, organisations, or similar

Heavy ions doping coupled with metallic nanoInclusions: An effective way to improve the thermoelectric performance of p-type layered cobalt oxide materials: 30th International Conference on Thermoelectrics-ICT2011
Period: 1 Jan 2011 → …
Ngo Van Nong (Speaker)
Department of Energy Conversion and Storage

Description
Place: Traverse City, Michigan, USA

Related external organisation

Unknown external organisation
Activity: Talks and presentations › Conference presentations

Recent Progress in Nanostructured Oxide TE Materials for Power Generation at High Temperatures: "Workshop on Advanced Materials Science and Nanotechnology"
Period: 1 Jan 2011 → …
Ngo Van Nong (Speaker)
Department of Energy Conversion and Storage

Description
Place: Hanoi, Vietnam

Related external organisation

Unknown external organisation
Activity: Talks and presentations › Conference presentations

Recent Progress in Nanostructured Thermoelectric Oxide Materials at Risø DTU: Workshop on Nanothermoelectrics
Period: 1 Jan 2011 → …
Ngo Van Nong (Speaker)
Department of Energy Conversion and Storage
Design and fabrication of broadband anti-reflection sub-wavelength periodic structure for solar cells

Period: 2010 → …
Francesco Pastorelli (Speaker)
Department of Energy Conversion and Storage
Functional organic materials

Renewable energy
27/06/2010 → 02/07/2010
Yokoama, Japan
Activity: Talks and presentations › Conference presentations

Period: 2010 → 2014
Duc-The Ngo (Reviewer)
Department of Energy Conversion and Storage
Imaging and Structural Analysis
Department of Micro- and Nanotechnology
Molecular Windows

I have worked for Materials Science and Engineering B, and other journals of Elsevier since 2010

A New Active Magnetic Regeneration (AMR) Prototype
Period: 16 Nov 2010
Kurt Engelbrecht (Invited speaker)
Department of Energy Conversion and Storage
Electrofunctional materials

European Integrated Center for the Development of New Metallic Alloys and Compounds
15/09/2010 → 18/09/2010
Dresden, Germany
Activity: Talks and presentations › Conference presentations

Oxygen permeation and chemical reactivity of alkaline earth doped cobaltite perovskites for membrane applications: VII Brazilian Electroceramics Symposium
Period: 26 Oct 2010
Vincenzo Esposito (Invited speaker)
Related event

IX Brazilian MRS meeting : The Brazilian Materials Research Society
24/10/2010 → 28/10/2010
Minais Gerais, Brazil
Activity: Talks and presentations › Conference presentations

UDTU Education in University Teaching at DTU
Anne Hauch (Participant)
Department of Energy Conversion and Storage
Applied Electrochemistry
Description
Participation in module 1-4 (all modules) in UDTU Education in University Teaching at DTU
UDTU - university teachers education

Related event

UDTU Education in University Teaching at DTU
02/08/2010 → 30/06/2011
Lyngby, Denmark
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

International Symposium on Metal-Hydrogen Systems
Period: 19 Jul 2010 → 23 Jul 2010
Didier Blanchard (Participant)
Department of Energy Conversion and Storage
Atomic scale modelling and materials
Description
Poster Presentation - Rotational and Translational diffusion in Calcium Borohydride from QENS and DFT
MH2010

Related event

12th International Symposium on Metal-Hydrogen Systems
19/07/2010 → 23/07/2010
Moscow, Russian Federation
Activity: Attending an event › Participating in or organising a conference

Cimtec 2010
Period: 18 Jun 2010
Hanne Lauritzen (Speaker)
Department of Energy Conversion and Storage
Functional organic materials
Fabrication and Processing of Polymer and Organic Solar Cells

Related event

Cimtec 2010: 5th Forum on New Materials
13/06/2010 → 18/10/2010
Montecatini Terme, Italy
Activity: Talks and presentations › Conference presentations

EERA Joint Programme on Energy Storage (External organisation)
Period: 1 Jan 2010
Allan Schröder Pedersen (Participant)
Department of Energy Conversion and Storage

Description
European collaboration among universities and research institutions

Body type: European
Degree of recognition: International

Related external organisation

EERA Joint Programme on Energy Storage
Activity: Membership › Membership of research networks or expert groups

Udstilling med plastsolceller
Period: 1 Jan 2009
Torben Damgaard Nielsen (Speaker)
Department of Energy Conversion and Storage
Applications, Patents and Innovation
Risø National Laboratory for Sustainable Energy
Solar Energy Programme

Description
Enhedslistens årsmøde

Related external organisation

Enhedslisten
Denmark
Activity: Talks and presentations › Talks and presentations in private or public companies and organisations

Institute of Physics (External organisation)
Period: 2008 → …
Duc-The Ngo (Participant)
Department of Energy Conversion and Storage
Imaging and Structural Analysis
Department of Micro- and Nanotechnology
Molecular Windows

Description
Member

I have been a member of Institute of Physics (IOP, UK) since 2008
DESIGN OF THE ELECTROCERAMICS FOR SOLID OXIDE FUEL CELL APPLICATIONS: PLAYING WITH CERIA: Nanotechnology: Controlled Processing of Nanoparticle Structures and Composites

Period: 7 Oct 2008

Vincenzo Esposito (Invited speaker)

Department of Energy Conversion and Storage
Ceramic Engineering & Science

Description
Session: Nanoparticle Sintering II

Related event
Materials Science & Technology Conference and Exhibition: MS&T08
05/10/2008 → 09/10/2008
Pittsburgh, Pennsylvania, United States
Activity: Talks and presentations › Conference presentations

European Fuel Cell Forum (External organisation)
Period: Dec 2007 → Jun 2008
Anke Hagen (Participant)

Department of Energy Conversion and Storage
Applied Electrochemistry

Description
Scientific Committee
Degree of recognition: International

Related external organisation
European Fuel Cell Forum
Obgarrdihalde 2, CH-6043, Luzern-Adligenswil, Switzerland
Activity: Membership › Membership of committees, commissions, boards, councils, associations, organisations, or similar

Influence of Sintering on Electrochemical Properties of Nanocrystalline Doped-Ceria: F5 - Nanostructured Metal Oxides: Processing and Applications

Period: 2 Nov 2006

Vincenzo Esposito (Invited speaker)

Department of Energy Conversion and Storage
Ceramic Engineering & Science
Documents:
Meet. Abstr.-2006-Esposito-1765

Related event
210th ECS meeting, Cancun, Mexico, Oct 29-Nov 3, 2006.
01/01/2006 → …
Cancun, Mexico
Activity: Talks and presentations › Conference presentations
Prizes:

4th International DHC+ Student Awards - 1st prize
Dominik Franjo Dominkovic (Recipient)
Department of Energy Conversion and Storage, Centre for IT-Intelligent Energy Systems in Cities

Description
The 1st prize award was achieved for a report dubbed "Large scale heat pumps as a link between intermittent electrical energy sources and district heating sector". The evaluation committee awarded three papers. As announced, the prize consists of a research contribution of EUR 1000, presentation of findings at the En+Eff International Trade Fair and Congress for Heating, Cooling and CHP in Frankfurt on 19-20 April 2016 and publishing the article in the International EuroHeat & Power magazine.

Details
Awarded date: Mar 2016
Degree of recognition: International
Granting Organisations: Euroheat & Power international association
Prize: Prizes, scholarships, distinctions

August-Wilhelm Scheer Visiting Professorship@TUM
Tejs Vegge (Recipient)
Department of Energy Conversion and Storage, Atomic scale modelling and materials

Details
Awarded date: 2016
Granting Organisations: Technical University of Munich
Prize: Prizes, scholarships, distinctions

Best Poster Award at the Sustain 2017
Gisele Alves dos Reis Benatto (Recipient), Nicholas Riedel (Recipient), Claire Mantel (Recipient), Sune Thorsteinsson (Recipient), Peter Behrendorff Poulsen (Recipient), Søren Forchhammer (Recipient), Kenn H. B. Frederiksen (Recipient), Jan Vedde (Recipient), Harsh Parikh (Recipient), Sergiu Spataru (Recipient) & Dezso Sera (Recipient)
Department of Photonics Engineering, Photovoltaic Materials and Systems, Organic Energy Materials, Coding and Visual Communication, Centre of Excellence for Silicon Photonics for Optical Communications

Description
Outdoor luminescence imaging strategies for drone-based PV array inspection

Details
Awarded date: 6 Dec 2017
Degree of recognition: International
Granting Organisations: Technical University of Denmark
event: Sustain 2017
Prize: Prizes, scholarships, distinctions

Elite-Forsk-rejsestipendium (EliteForsk travel grant)
Dominik Franjo Dominkovic (Recipient)
Department of Energy Conversion and Storage, Centre for IT-Intelligent Energy Systems in Cities

Description
Awarded with the scholarship for the purpose of visiting different research groups. It will be used to finance the guest research stay at Energy Research Institute at Nanyang Technological University in Singapore and for the guest research stay at National Renewable Energy Laboratory (NREL) in Colorado, the USA.

Details
Awarded date: 23 Feb 2017
Degree of recognition: National
Granting Organisations: Ministry of Higher Education and Science
Prize: Prizes, scholarships, distinctions

Ellen and Hans Hermers Award 2015
Tejs Vegge (Recipient)
Center for Atomic-scale Materials Design, Department of Energy Conversion and Storage, Atomic scale modelling and materials

**Description**
The Foundation is managed by Rector of the University of Copenhagen, Prof. Ralf Hemmingsen, the Dean of the Faculty of Sciences at University of Copenhagen, Prof. John Renner Hansen, and the President of the Technical University of Denmark, Prof. Anders O. Bjarklev. The foundation awards honorary grants (unsolicited).

**Details**
Awarded date: 26 Jan 2015
Granting Organisations: Ellen and Hans Hermers Foundation
Prize: Prizes, scholarships, distinctions

**Member of the Danish Academy of Technical Sciences (ATV)**
Tejs Vegge (Recipient)
Center for Atomic-scale Materials Design, Department of Energy Conversion and Storage, Atomic scale modelling and materials

**Details**
Awarded date: May 2014
Granting Organisations: Danish Academy of Technical Sciences (ATV)
Prize: Prizes, scholarships, distinctions

**PhD Supervisor the year 2017**
Tejs Vegge (Recipient)
Department of Energy Conversion and Storage, Atomic scale modelling and materials

**Description**
PhD Supervisor of the year at DTU

**Details**
Awarded date: 27 Oct 2017
Granting Organisations: Technical University of Denmark
Prize: Prizes, scholarships, distinctions

**Third Price EFC17 Best Paper Awards**
Søren Højgaard Jensen (Recipient), Hendrik Langnickel (Recipient), Nils Hintzen (Recipient), Ming Chen (Recipient), Xiufu Sun (Recipient), Anne Hauch (Recipient), Giacomo Butera (Recipient) & Lasse Røngaard Clausen (Recipient)
Department of Energy Conversion and Storage, Applied Electrochemistry, Mixed Conductors, Department of Mechanical Engineering, Thermal Energy

**Description**
Third price for the paper: “Reversible Operation using Carbonaceous Gasses of a 30-cell Solid Oxide Cell Stack”

The awards are given to the best papers submitted to the EFC17 conference and that report the most important insights and progress within the broad field of hydrogen and fuel cell technologies. The awards are sponsored by the EFC17 conference. All nominations are judged by an independent Best Paper Selection Committee.

**Details**
Awarded date: 13 Dec 2017
Degree of recognition: International
event: 7th European Fuel Cell Piero Lunghi Conference
Prize: Prizes, scholarships, distinctions

**Press clippings:**

**Nyt batteri kan oplades på ét minut og give 800 km rækkevidde**
Tejs Vegge
16/11/2017
Atomic scale modelling and materials, Department of Energy Conversion and Storage

**Media contribution (1)**
Nyt batteri kan oplades på ét minut og give 800 km rækkevidde
16/11/2017
www.ing.dk, Denmark, Web
https://ing.dk/artikel/nyt-batteri-kan-oplades-paa-minut-give-800-km-raekkevidde-208620
Tejs Vegge
Press / Media

The Race to Build Better Batteries
Tejs Vegge
01/11/2017
Atomic scale modelling and materials, Department of Energy Conversion and Storage

Sådan får du dit batteri til at holde længere
Tejs Vegge
24/10/2017
Atomic scale modelling and materials, Department of Energy Conversion and Storage

Elektriske fly
Tejs Vegge
16/06/2017
Atomic scale modelling and materials, Department of Energy Conversion and Storage

Rumforskning: Han skal sikre astronauter en returbillet fra Mars
Christopher R. Graves
17/05/2017

Description
Article in Jyllands Posten about Christopher Graves's involvement in a NASA project that will send a CO2 electrolyzer to Mars on the rover in 2020.
Following is the link to the article. A PDF of the full could be uploaded if there was an attachment option.
Applied Electrochemistry, Department of Energy Conversion and Storage

Rumforskning: Han skal sikre astronauter en returbillet fra Mars
17/05/2017
Jyllands Posten (National), Denmark, Print
Batterirevolutionen lader vente på sig
Tejs Vegge
03/05/2017
Atomic scale modelling and materials, Department of Energy Conversion and Storage

Media contribution (1)

Batterirevolutionen lader vente
03/05/2017
Nordea Invest Magasin, Denmark, Web
http://nordeainvesmagasinet.dk/artikler/batterirevolutionen-lader-vente-pa-sig
Tejs Vegge
Press / Media

Mercedes satser stort på produktion af højeffektive batterier
Tejs Vegge
27/04/2017
Atomic scale modelling and materials, Department of Energy Conversion and Storage

Media contribution (1)

Mercedes satser stort på produktion af højeffektive batterier
27/04/2017
DI Energi årsmagasin 2017, Denmark, Web
http://Mercedes satser stort på produktion af højeffektive batterier
Tejs Vegge
Press / Media

Ny kemi i batterier øger muligheden for at lagre grøn energi
Tejs Vegge
20/02/2017
Atomic scale modelling and materials, Department of Energy Conversion and Storage

Media contribution (1)

Ny kemi i batterier øger muligheden for at lagre grøn energi
20/02/2017
Ingeniøren, Denmark, Web
https://ing.dk/artikel/ny-kemi-batterier-oeger-muligheden-at-lagre-groen-energi-193977
Tejs Vegge
Press / Media

Derfor fryser din mobil sig selv ihjel i kulden
Tejs Vegge
07/01/2017
Atomic scale modelling and materials, Department of Energy Conversion and Storage

Media contribution (1)

Derfor fryser din mobil sig selv ihjel i kulden
07/01/2017
www.tv2.dk, Denmark, Web
http://livsstil.tv2.dk/forbrug/2017-01-06-derfor-fryser-din-mobil-sig-selv-ihjel-i-kulden
Tejs Vegge
Press / Media
Ingeniøren - Året Rundt 2016: Lang vej til nye batteriteknologier
Tejs Vegge
31/12/2016
Atomic scale modelling and materials, Department of Energy Conversion and Storage

Media contribution (1)

Ingeniøren - Året Rundt 2016: Lang vej til nye batteriteknologier
31/12/2016
Ingeniøren, Print
https://ing.dk/artikel/lang-vej-nye-batteriteknologier-190102
Tejs Vegge
Department of Energy Conversion and Storage, Atomic scale modelling and materials
Press / Media

DHC+ newsletter: Interview with Dominik Franjo Dominković, winner of the 4th International DHC+ Student Awards
Dominik Franjo Dominkovic
10/10/2016

Description
An interview with the several questions concerning the participation in the DHC+ Student Awards Competition
Department of Energy Conversion and Storage, Centre for IT-Intelligent Energy Systems in Cities

Media contribution (1)

DHC+ newsletter: Interview with Dominik Franjo Dominković, winner of the 4th International DHC+ Student Awards
10/10/2016
DHC+ Technology Platform, Web
DHC+ Technology Platform
Dominik Franjo Dominkovic
Department of Energy Conversion and Storage, Centre for IT-Intelligent Energy Systems in Cities
Press / Media

Eksperter: Samsungs brandfarlige batterier er bekymrende
Tejs Vegge
11/09/2016
Atomic scale modelling and materials, Department of Energy Conversion and Storage

Media contribution (1)

Eksperter: Samsungs brandfarlige batterier er bekymrende
11/09/2016
www.dr.dk, Web
https://www.dr.dk/nyheder/indland/eksperter-samsungs-brandfarlige-batterier-er-bekymrende
Tejs Vegge
Atomic scale modelling and materials, Department of Energy Conversion and Storage
Press / Media

Millionærklubben
Tejs Vegge
04/05/2016
Atomic scale modelling and materials, Department of Energy Conversion and Storage

Media contribution (1)

Millionærklubben
04/05/2016
Radio24Syv, Radio
1 hour
http://www.radio24syv.dk/programmer/millionaerklubben/13444666/millionaerklubben-04-05-2016/
Tejs Vegge
Department of Energy Conversion and Storage, Atomic scale modelling and materials
Press / Media
Skimmelsvamp gør batterier bedre?
Tejs Vegge
17/04/2016
Atomic scale modelling and materials, Department of Energy Conversion and Storage

Media contribution (1)

Skimmelsvamp gør batterier bedre?
17/04/2016
www.videnskab.dk, Web
http://videnskab.dk/miljo-naturvidenskab/skimmelsvamp-kan-gore-batterier-bedre
Tejs Vegge
Department of Energy Conversion and Storage, Atomic scale modelling and materials
Press / Media

Energirevolutionen er lige om hjørnet
Tejs Vegge
08/03/2016
Atomic scale modelling and materials, Department of Energy Conversion and Storage

Media contribution (1)

Energirevolutionen er lige om hjørnet
08/03/2016
Berlingske Business, Print
http://www.business.dk/energi/energirevolutionen-er-lige-om-hjoernet
Tejs Vegge
Department of Energy Conversion and Storage, Atomic scale modelling and materials
Press / Media

Bliver batterier ikke snart bedre?
Tejs Vegge
03/03/2016
Atomic scale modelling and materials, Department of Energy Conversion and Storage

Media contribution (1)

Bliver batterier ikke snart bedre?
03/03/2016
www.videnskab.dk, Web
http://videnskab.dk/sporg-videnskaben/bliver-batterier-ikke-snart-bedre
Tejs Vegge
Department of Energy Conversion and Storage, Atomic scale modelling and materials
Press / Media

Bill Gates forgylder tre enegriteknologier
Tejs Vegge
04/12/2015
Atomic scale modelling and materials, Department of Energy Conversion and Storage, Center for Atomic-scale Materials Design

Media contribution (1)

Bill Gates forgylder tre enegriteknologier
04/12/2015
Ingeniøren, Print
Tejs Vegge
Center for Atomic-scale Materials Design, Department of Energy Conversion and Storage, Atomic scale modelling and materials
Press / Media
Bill Gates med energi nummer 1: Flowbatterier
Tejs Vegge
04/12/2015
Atomic scale modelling and materials, Department of Energy Conversion and Storage, Center for Atomic-scale Materials Design

Media contribution (1)

Bill Gates med energi nummer 1: Flowbatterier
Tejs Vegge
03/12/2015
Ingeniøren, Print
Tejs Vegge
Center for Atomic-scale Materials Design, Department of Energy Conversion and Storage, Atomic scale modelling and materials
Press / Media

Bill Gates med energi nummer 1: Flowbatterier
Tejs Vegge
03/12/2015
www.ing.dk, Web
Tejs Vegge
Center for Atomic-scale Materials Design, Department of Energy Conversion and Storage, Atomic scale modelling and materials
Press / Media

Batterier der virkelig batter
Tejs Vegge
27/10/2015
Atomic scale modelling and materials, Department of Energy Conversion and Storage, Center for Atomic-scale Materials Design

Media contribution (1)

Batterier der virkelig batter
27/10/2015
Børsen Gadget, Print
Tejs Vegge
Center for Atomic-scale Materials Design, Department of Energy Conversion and Storage, Atomic scale modelling and materials
Press / Media

So ein Ding: Solstrøm og Megabatterier
Tejs Vegge
25/10/2015
Atomic scale modelling and materials, Department of Energy Conversion and Storage, Center for Atomic-scale Materials Design

Media contribution (1)

So ein Ding: Solstrøm og Megabatterier
25/10/2015
DR2, Television
Danmarks Radio
Tejs Vegge
Center for Atomic-scale Materials Design, Department of Energy Conversion and Storage, Atomic scale modelling and materials
Press / Media
Tejs Vegge
Center for Atomic-scale Materials Design, Department of Energy Conversion and Storage, Atomic scale modelling and materials, Department of Physics
Press / Media

Nyt batteri kan forsyne dit hus med strøm
Tejs Vegge
01/05/2015
Department of Physics, Atomic scale modelling and materials, Department of Energy Conversion and Storage, Center for Atomic-scale Materials Design

Media contribution (1)

Nyt batteri kan forsyne dit hus med strøm
01/05/2015
TV2 News, Television
Tejs Vegge
Center for Atomic-scale Materials Design, Department of Energy Conversion and Storage, Atomic scale modelling and materials, Department of Physics
Press / Media

Forbedring af batterier er et langt, sejt træk
Tejs Vegge
17/04/2015
Department of Physics, Atomic scale modelling and materials, Department of Energy Conversion and Storage, Center for Atomic-scale Materials Design

Media contribution (1)

Forbedring af batterier er et langt, sejt træk
17/04/2015
Ingeniøren, Print
Tejs Vegge
Center for Atomic-scale Materials Design, Department of Energy Conversion and Storage, Atomic scale modelling and materials, Department of Physics
Press / Media

Højlunds Helte: Tre DTU'ers løsninger på fremtidens problemer med CO2
Anne Hauch
15/03/2015

Description
Three researchers from DTU Energy participate in the Sunday morning programme ‘Højlund’s Heroes’ on the radio channel Radio24syv. They go live in the radio at 08:25 to approx. 09:00 on Sunday morning, 15 March.

In the programme Højlund’s Heroes, PhD student Søren Lyng Ebbehøj, senior researcher Anne Hauch and Professor Jens Oluf Jensen will talk about the following energy research topic: How do we get fuel in the future?

Højlund’s Heroes is a programme that tells the positive story. The media landscape is fraught with problems, concerns and disasters, but every time there is something to worry about, there are also some ambitious people trying to find the solution. The objective of Højlund’s Heroes is to focus on those people and their work.

Energy is very important in climate perspective and policy perspectives, and many are worried about how we get energy in the future. DTU Energy has been invited to talk about its research in energy technologies, because - as journalist Grethe Højlund says - there's something inspiring about people moving into the unknown territory to find the solutions of tomorrow.

You can follow our researchers (in Danish) at http://www.radio24syv.dk/programmer/hoejlunds-helte/ this Sunday morning from 08.25 in the morning.

Subject
CO2 capture, electrolysis, fuel cells - Manufacturing Green Fuels from Renewable Energy
Applied Electrochemistry, Department of Energy Conversion and Storage
Media contribution (1)

Højlunds Helte: Tre DTU'ers løsninger på fremtidens problemer med CO2
15/03/2015
Radio24syv, Radio
Danmarks Radio
25 minutes
The interview of Søren Lyng Ebbehøj, I and Jens Oluf Jensen starts approximately after 24 minutes of the program
Anne Hauch
Department of Energy Conversion and Storage, Applied Electrochemistry
Press / Media

Article in ComputerWorld (DK)
Michael Corazza
02/01/2015
Department of Energy Conversion and Storage, Functional organic materials

Media contribution (1)

Article in ComputerWorld (DK)
02/01/2015
Print
http://www.computerworld.dk/art/232794/risoe-forsker-open-source-er-et-lystvaerk
Michael Corazza
Department of Energy Conversion and Storage, Functional organic materials
Press / Media

Nyt flowbatteri har lovende fremtid
Tejs Vegge
23/06/2014
Atomic scale modelling and materials, Department of Energy Conversion and Storage, Center for Atomic-scale Materials Design

Media contribution (1)

Nyt flowbatteri har lovende fremtid
23/06/2014
Ingeniøren, Print
Tejs Vegge
Center for Atomic-scale Materials Design, Department of Energy Conversion and Storage, Atomic scale modelling and materials
Press / Media

Elektrokemi kan ændre vædning mellem metal og keramik: Forskere på DTU Energikonvertering har opdaget, at elektrokemi kan ændre vædningen mellem metal og keramik.
Janet Jonna Bentzen
01/01/2014
Department of Energy Conversion and Storage, Imaging and Structural Analysis

Media contribution (1)

Elektrokemi kan ændre vædning mellem metal og keramik: Forskere på DTU Energikonvertering har opdaget, at elektrokemi kan ændre vædningen mellem metal og keramik.
01/01/2014
Dansk Kemi, Print
Kasper H. Skovse
http://techmedia.swiflet.com/tm/dak/73/1/
Janet Jonna Bentzen
Department of Energy Conversion and Storage, Imaging and Structural Analysis

Relations

Research outputs:
Electrochemistry Unlocks Wettability: Epitaxial Growth of Oxide Nanoparticles on Rough Metallic Surfaces
Strom & Gas Synergie
Anke Hagen
01/01/2013
Applied Electrochemistry, Department of Energy Conversion and Storage

Media contribution (1)

Strom & Gas Synergie
01/01/2013
Sonnenenergie, Print
E. Kuehnle
Anke Hagen
Department of Energy Conversion and Storage, Applied Electrochemistry
Press / Media

Anastasia Aleksandrovna Permyakova
01/01/2012

Description
http://emagstudio.win.dtu.dk/E-books/DTU-Avisen/DTUavis0112/#/20/
Energy and Materials, Department of Energy Conversion and Storage, Proton conductors

Media contribution (1)

01/01/2012
DTU Avisen, Print
Charlotte Malasse
http://emagstudio.win.dtu.dk/E-books/DTU-Avisen/DTUavis0112/#/20/
Anastasia Aleksandrovna Permyakova
Department of Energy Conversion and Storage, Proton conductors, Energy and Materials
Press / Media

Højeffektive brændselsceller
Trine Klemensø
01/01/2010

Description
SOFC project promotion film for The Danish National Advanced Technology Foundation.
Ceramic Engineering & Science, Department of Energy Conversion and Storage

Media contribution (1)

Højeffektive brændselsceller
01/01/2010
Web
Højteknologifonden
10 min
Trine Klemensø
Department of Energy Conversion and Storage, Ceramic Engineering & Science
Press / Media