Acoustic Streaming and Its Suppression in Inhomogeneous Fluids

We present a theoretical and experimental study of boundary-driven acoustic streaming in an inhomogeneous fluid with variations in density and compressibility. In a homogeneous fluid this streaming results from dissipation in the boundary layers (Rayleigh streaming). We show that in an inhomogeneous fluid, an additional nondissipative force density acts on the fluid to stabilize particular inhomogeneity configurations, which markedly alters and even suppresses the streaming flows. Our theoretical and numerical analysis of the phenomenon is supported by ultrasound experiments performed with inhomogeneous aqueous iodixanol solutions in a glass-silicon microchip.

General information
State: Published
Organisations: Department of Physics, Biophysics and Fluids, Lund University
Authors: Karlsen, J. T. (Intern), Qiu, W. (Intern), Augustsson, P. (Ekstern), Bruus, H. (Intern)
Number of pages: 6
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information
Journal: Physical Review Letters
Volume: 120
Issue number: 5
Article number: 054501
ISSN (Print): 0031-9007
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
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Original language: English
Electronic versions:

Untitled.pdf
A General Microscopic Traffic Model Yielding Dissipative Shocks
We consider a general microscopic traffic model with a delay. An algebraic traffic function reduces the equation to the Aw-Rascle microscopic model while a sigmoid function gives the standard “follow the leader”. For zero delay we prove that the homogeneous solution is globally stable. For a positive delay, it becomes unstable and develops dispersive and dissipative shocks. These are followed by a finite time singularity for the algebraic traffic function and by kinks for the sigmoid function.

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Department of Physics, Plasma Physics and Fusion Energy, Dynamical Systems, Center for Intelligent Drug Delivery and Sensing Using Microcontainers and Nanomechanics, Bogolyubov Institute for Theoretical Physics, INSA Rouen
Authors: Gaididei, Y. B. (Ekstern), Caputo, J. G. (Ekstern), Christiansen, P. L. (Intern), Rasmussen, J. J. (Intern), Sørensen, M. (Intern)
Pages: 375-382
Publication date: 2018

A laser heating facility for energy-dispersive X-ray absorption spectroscopy
A double-sided laser heating setup for diamond anvil cells installed on the ID24 beamline of the ESRF is presented here. The setup geometry is specially adopted for the needs of energy-dispersive X-ray absorption spectroscopic (XAS) studies of materials under extreme pressure and temperature conditions. We illustrate the performance of the facility with a study on metallic nickel at 60 GPa. The XAS data provide the temperature of the melting onset and quantitative information on the structural parameters of the first coordination shell in the hot solid up to melting.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, European Synchrotron Radiation Facility
Authors: Kantor, I. (Intern), Marini, C. (Ekstern), Mathon, O. (Ekstern), Pascarelli, S. (Ekstern)
Number of pages: 13
Publication date: 2018
Main Research Area: Technical/natural sciences
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 0.858 SJR 0.585 CiteScore 1.32
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
Scopus rating (2010): SJR 1.218 SNIP 1.405
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.001 SNIP 1.061
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.274 SNIP 1.344
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.922 SNIP 1.023
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.153 SNIP 1.297
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.883 SNIP 1.044
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.13 SNIP 1.393
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 0.994 SNIP 1.301
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 1.02 SNIP 1.015
Scopus rating (2001): SJR 1.13 SNIP 1.301
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 1.022 SNIP 1.051
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 0.979 SNIP 1.043

Original language: English
Laser applications, X-ray absorption spectroscopy, Transition, Diamond-anvil, Absorption spectra
DOIs:
Ambient Pressure Hydrodesulfurization of Refractory Sulfur Compounds in Highly Sensitive μ-Reactor Platform Coupled to a Time-of-Flight Mass Spectrometer

Tightened restrictions call for cleaner transportation fuels to minimize environmental and societal problems caused by the presence of sulfur in transportation fuels. This emphasizes the need for new and better catalysts in the field of hydrodesulfurization (HDS), which aims at removing the refractory sulfur from different petroleum streams mostly found in the form of the alkyl-substituted dibenzothiophenes (β-DBTs). In this work we demonstrate how a setup dedicated to testing minute amounts (nanogram) of well-defined catalytic systems in μ-reactors can be used in the gas-phase HDS of the model compounds DBT and 4,6-dimethyldibenzothiophene (4,6-DMDBT) and the reaction pathways revealed by time-of-flight mass spectrometry. Specifically, we investigate HDS of DBT and 4,6-DMDBT on mass-selected Pt nanoparticles and show that only the direct desulfurization products are formed. The setup is a means to bridge the gap between structural characterization of model catalysts and their related activity in the HDS of DBT and 4,6-DMDBT.
Anisotropy enhanced X-ray scattering from solvated transition metal complexes

Time-resolved X-ray scattering patterns from photoexcited molecules in solution are in many cases anisotropic at the ultrafast time scales accessible at X-ray free-electron lasers (XFELs). This anisotropy arises from the interaction of a linearly polarized UV-Vis pump laser pulse with the sample, which induces anisotropic structural changes that can be captured by femtosecond X-ray pulses. In this work, a method for quantitative analysis of the anisotropic scattering signal arising from an ensemble of molecules is described, and it is demonstrated how its use can enhance the structural sensitivity of the time-resolved X-ray scattering experiment. This method is applied on time-resolved X-ray scattering patterns measured upon photoexcitation of a solvated di-platinum complex at an XFEL, and the key parameters involved are explored. It is shown that a combined analysis of the anisotropic and isotropic difference scattering signals in this experiment allows a more precise determination of the main photoinduced structural change in the solute, i.e. the change in Pt-Pt bond length, and yields more information on the excitation channels than the analysis of the isotropic scattering only. Finally, it is discussed how the anisotropic transient response of the solvent can enable the determination of key experimental parameters such as the instrument response function.

General information

State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Department of Chemistry, Department of Electric Power Engineering, University of Iceland, SLAC National Accelerator Laboratory, Technical University of Denmark
Pages: 306-315
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information

Journal: Journal of Synchrotron Radiation
Volume: 25
Issue number: 2
ISSN (Print): 0909-0495
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Anomalous behavior of the excited state of the A exciton in bulk WS2

Results of optical spectroscopy studies on bulk 2H-WS2 at energies close to its direct band gap are presented. Reflectance and absorption measurements at low temperature show only one dominant feature due to the A exciton of bulk WS2 at similar to 2.02 eV. However, a laser-modulated photoreflectance spectrum looks quite different, revealing a second even stronger feature A* similar to 62 meV above A. The relative intensity of these two features is shown to
change significantly in a lateral electroreflectance measurement with electric field applied perpendicular to the c axis of WS2. The experimental results are analyzed by comparison with many-body perturbation theory calculations, including the solutions of the Bethe-Salpeter equation. A* is identified as the first excited state of the A exciton, that is, A(n = 2). The anomalous behavior of A* is explained by its distinct wave function spread along the c axis, the direction of weak van der Waals bonding, which makes it more susceptible to perturbations. Our ab initio calculations suggest that the A exciton in the ground state has a two-dimensional (2D) nature with a large binding energy E_b, in fair agreement with E_b similar to 90 +/- 20 meV estimated from a temperature-dependent reflectance study. The applicability of the 2D hydrogenic Wannier-Mott model for the exciton spectrum of a layered semiconductor like bulk WS2 is discussed.

General information
State: Published
Organisations: Department of Physics, Theoretical Atomic-scale Physics, Tata Institute of Fundamental Research
Authors: Jindal, V. (Ekstern), Bhuyan, S. (Ekstern), Deilmann, T. (Intern), Ghosh, S. (Ekstern)
Number of pages: 6
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information
Journal: Physical Review B
Volume: 97
Issue number: 4
Article number: 045211
ISSN (Print): 1098-0121
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
A novel method to remove the background from x-ray diffraction signal

The first step that is required to extract the correct information from a two-dimensional (2D) diffraction signature is to remove the background accurately. However, direct background subtraction inevitably overcorrects the signal as it does not take into account the attenuation by the sample. Other traditional background removal methods, such as the rolling ball technique, can separate sharp diffraction peaks of crystalline materials from their background. These methods are unsuitable for biological tissue, which is amorphous and does not have sharp diffraction peaks. This technical note proposes a novel method that combines peak fitting and experimental results to estimate the background for 2D XRD signals.
A spectral geometric model for Compton single scatter in PET based on the single scatter simulation approximation: Paper

We investigate the idealized mathematical model of single scatter in PET for a detector system possessing excellent energy resolution. The model has the form of integral transforms estimating the distribution of photons undergoing a single Compton scattering with a certain angle. The total single scatter is interpreted as the volume integral over scatter points that constitute a rotation body with a football shape, while single scattering with a certain angle is evaluated as the surface integral over the boundary of the rotation body. The equations for total and sample single scatter calculations are derived using a single scatter simulation approximation. We show that the three-dimensional slice-by-slice filtered backprojection algorithm is applicable for scatter data inversion provided that the attenuation map is assumed to be constant. The results of the numerical experiments are presented.

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Department of Physics, Neutrons and X-rays for Materials Physics, Scientific Computing, Institute of Computational Mathematics and Mathematical Geophysics
Authors: Kazantsev, I. (Ekstern), Olsen, U. L. (Intern), Poulsen, H. F. (Intern), Hansen, P. C. (Intern)
Number of pages: 15
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information
Journal: Inverse Problems
Volume: 34
Issue number: 2
Article number: 024002
Growing concern regarding the sustainability of the chemical industry has driven the development of more efficient catalytic reactions. First-generation estimates of catalyst viability are based on crustal abundance, which has severe limitations. Herein, we propose a second-generation approach to predicting the viability of novel catalysts prior to industrial implementation to benefit the global chemical industry. Using this prediction, we found that a correlation exists between catalyst consumption and the annual production or price of the catalyst element for 11 representative industrial catalytic processes. Based on this correlation, we have introduced two new descriptors for catalyst viability, namely, catalyst...
consumption to availability ratio per annum (CCA) and consumed catalyst cost to product value ratio per annum (CCP).

Based on evaluations of CCA and CCP for selected industrial reactions, we have grouped catalysts from the case studies according to viability, allowing the identification of general limits of viability based on CCA and CCP. Calculating the CCA and CCP and their comparing with the general limits of viability provides researchers with a novel framework for evaluating whether the cost or physical availability of a new catalyst could be limiting. We have extended this analysis to calculate the predicted limits of economically viable production and product cost for new catalysts.
Bayesian Integrated Data Analysis of Fast-Ion Measurements by Velocity-Space Tomography

Bayesian integrated data analysis combines measurements from different diagnostics to jointly measure plasma parameters of interest such as temperatures, densities, and drift velocities. Integrated data analysis of fast-ion measurements has long been hampered by the complexity of the strongly non-Maxwellian fast-ion distribution functions. This has recently been overcome by velocity-space tomography. In this method two-dimensional images of the velocity distribution functions consisting of a few hundreds or thousands of pixels are reconstructed using the available fast-ion measurements. Here we present an overview and current status of this emerging technique at the ASDEX Upgrade tokamak and the JET tokamak based on fast-ion D-alpha spectroscopy, collective Thomson scattering, gamma-ray and neutron emission spectrometry, and neutral particle analyzers. We discuss Tikhonov regularization within the Bayesian framework. The implementation for different types of diagnostics as well as the uncertainties are discussed, and we highlight the importance of integrated data analysis of all available detectors.

General information
State: Accepted/In press
Organisations: Department of Physics, Plasma Physics and Fusion Energy, University of Milano Bicocca, Max-Planck-Institut fur Plasmaphysik, Uppsala University, Rutherford Appleton Laboratory, Culham Science Centre, Aalto University, Consiglio Nazionale delle Ricerche
Number of pages: 14
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information
Journal: Fusion Science and Technology
ISSN (Print): 1536-1055
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 0.982 SJR 0.383 CiteScore 0.96
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 0.57 SJR 0.423 SNIP 0.728
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.411 SNIP 0.759 CiteScore 0.65
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.357 SNIP 0.536 CiteScore 0.46
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.382 SNIP 0.582 CiteScore 0.56
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.448 SNIP 0.704 CiteScore 0.54
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.617 SNIP 1.195 CiteScore 0.93
ISI indexed (2011): ISI indexed yes
We present an extensive set of surface and chemisorption energies calculated using state of the art many body perturbation theory. In the first part of the paper we consider 10 surface reactions in the low coverage regime where experimental data is available. Here the random phase approximation (RPA) is found to yield high accuracy for both adsorption and surface energies. In contrast, all the considered density functionals fail to describe both quantities accurately. This establishes the RPA as a universally accurate method for surface science. In the second part, we use the RPA to construct a database of 200 high quality adsorption energies for reactions involving OH, CH, NO, CO, N₂, N, O, and H over a wide range of 3d, 4d, and 5d transition metals. Due to the significant computational demand, these results are obtained in the high coverage regime where adsorbate-adsorbate interactions can be significant. RPA is compared to the more advanced renormalized adiabatic LDA (rALDA) method for a subset of the reactions, and they are found to describe the adsorbate-metal bond as well as adsorbate-adsorbate interactions similarly. The RPA results are compared to a range of standard density functional theory methods typically employed for surface reactions representing the various rungs on Jacob's ladder. The deviations are found to be highly functional, surface, and reaction dependent. Our work establishes the RPA and rALDA methods as universally accurate full ab initio methods for surface science where accurate experimental data is scarce. The database is freely available via the Computational Materials Repository (CMR).
Carbon catalysts for electrochemical hydrogen peroxide production in acidic media

Hydrogen peroxide is a commodity chemical, as it is an environmentally friendly oxidant. The electrochemical production of H₂O₂ from oxygen and water by the reduction of oxygen is of great interest, as it would allow the decentralized, on-site, production of pure H₂O₂. The ability to run the reaction in an acidic electrolyte with high performance is particularly important, as it would allow the use of polymer solid electrolytes and the production of pH-neutral hydrogen peroxide. Carbon catalysts, which are cheap, abundant, durable and can be highly selective show promise as potential catalysts for such systems. In this work, we examine the electrocatalytic performance and properties of seven commercially available carbon materials for H₂O₂ production by oxygen electroreduction. We show that the faradaic efficiencies for the reaction lie in a wide range of 18-82% for different carbon catalysts. In order to determine the cause of these differences, we
employ prompt gamma ray/neutron activation analysis and XPS measurements to assess the contribution of heteroatoms and defects, as well as low temperature N₂-adsorption and transmission electron microscopy to elucidate the particle size, shape, BET surface area and porosity. We find that the surface oxygen groups, nitrogen and sulphur content display effects that are not straightforward, because their chemical state is likely significant. The metal content (when present in the order of magnitude of ~10 ppm) is not a straightforward indicator of the electrocatalytic performance for this reaction. XPS and BET data indicate that carbons displaying high selectivities for the 2-electron process contain more aliphatic-like, “defect” structures on the surface.

**General information**

*State:* Published  
*Organisations:* Department of Physics, Experimental Surface and Nanomaterials Physics, Technische Universität München  
*Authors:* Čolić, V. (Intern), Yang, S. (Intern), Révay, Z. (Ekstern), Stephens, I. E. (Intern), Chorkendorff, I. (Intern)  
*Pages:* 192-202  
*Publication date:* 2018  
*Main Research Area:* Technical/natural sciences

**Publication information**

*Journal:* Electrochimica Acta  
*Volume:* 272  
*ISSN (Print):* 0013-4686  
*Ratings:*  
BFI (2018): BFI-level 2  
Web of Science (2018): Indexed yes  
BFI (2017): BFI-level 2  
Scopus rating (2017): SJR 1.439 SNIP 1.101 CiteScore 5.01  
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
Comprehensive cluster-theory analysis of the magnetic structures and excitations in CoCl$_2$·2H$_2$O

The magnetic properties of CoCl$_2$·2H$_2$O are analyzed in the mean-field/random-phase approximation using a basis of clusters with four spins along the c-axis chains of Co ions. The model gives a unifying account of the bulk properties, the spin waves, and the higher-order cluster-spin excitations. The theory describes accurately the neutron scattering measurements of the excited doublet of the S = 3/2 Co$^{3+}$ ions in both the antiferromagnetic and the paramagnetic phases. The theory has been applied by Larsen et al. [Phys. Rev. B 96, 174424 (2017)] for analyzing the quantum phase transition at a transverse field of 160 kOe and is found to agree closely with their observations.

General information
State: Published
Organisations: Department of Physics, University of Copenhagen
Authors: Jensen, J. (Ekstern), Larsen, J. (Intern), Hansen, U. B. (Ekstern)
Number of pages: 9
Publication date: 2018
Main Research Area: Technical/natural sciences
Computational Screening of Light-absorbing Materials for Photoelectrochemical Water Splitting
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
Chapter: 3
Main Research Area: Technical/natural sciences
DOIs: 10.1039/9781782629863-00062
Publication: Research - peer-review › Book chapter – Annual report year: 2018

Conjugated Polymers and Oligomers: Structural and Soft Matter Aspects
This book identifies modern topics and current trends of structural and soft matter aspects of conjugated polymers and oligomers. Each chapter recognizes an active research line where structural perspective dominates research and therefore the book covers fundamental aspects of persistent conjugated polymer backbone, water soluble conjugated polyelectrolytes and surfactants, conjugated molecules and biomolecules and DNA and the advanced use of synchrotron radiation and electron microscopy to find out structural details in conjugated molecule films and devices as well as under ambient and extreme conditions.

General information
State: Accepted/In press
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics
Authors: Knaapila, M. (ed.) (Intern)
Publication date: 2018

Publication information
Publisher: World Scientific Publishing Co
ISBN (Print): 978-981-3225-75-6
Original language: English
Series: Materials and Energy
Volume: 9
Main Research Area: Technical/natural sciences
Publication: Research - peer-review › Book – Annual report year: 2018

Continuous-variable protocol for oblivious transfer in the noisy-storage model
Cryptographic protocols are the backbone of our information society. This includes two-party protocols which offer protection against distrustful players. Such protocols can be built from a basic primitive called oblivious transfer. We present and experimentally demonstrate here a quantum protocol for oblivious transfer for optical continuous-variable systems, and prove its security in the noisy-storage model. This model allows us to establish security by sending more quantum signals than an attacker can reliably store during the protocol. The security proof is based on uncertainty relations which we derive for continuous-variable systems, that differ from the ones used in quantum key distribution. We experimentally demonstrate in a proof-of-principle experiment the proposed oblivious transfer protocol for various channel losses by using entangled two-mode squeezed states measured with balanced homodyne detection. Our work enables the implementation of arbitrary two-party quantum cryptographic protocols with continuous-variable communication systems.
Contributed review: camera-limits for wide-field magnetic resonance imaging with a nitrogen-vacancy spin sensor

Sensitive, real-time optical magnetometry with nitrogen-vacancy centers in diamond relies on accurate imaging of small (<10⁻²) fractional fluorescence changes across the diamond sample. We discuss the limitations on magnetic field sensitivity resulting from the limited number of photoelectrons that a camera can record in a given time. Several types of camera sensors are analyzed, and the smallest measurable magnetic field change is estimated for each type. We show that most common sensors are of a limited use in such applications, while certain highly specific cameras allow achieving nanotesla-level sensitivity in 1 s of a combined exposure. Finally, we demonstrate the results obtained with a lock-in camera that paves the way for real-time, wide-field magnetometry at the nanotesla level and with a micrometer resolution.
Corrections to "Intermetallic GaPd2 Nanoparticles on SiO2 for Low-Pressure CO2 Hydrogenation to Methanol: Catalytic Performance and In Situ Characterization"
Correlating charge transport to structure in deconstructed diketopyrrolopyrrole oligomers: A case study of a monomer in field-effect transistors

Copolymers based on diketopyrrolopyrrole (DPP) cores have attracted a lot of attention due to their high p-type as well as n-type carrier mobilities in organic field-effect transistors (FETs) and high power conversion efficiencies in solar cell structures. We report the structural and charge transport properties of n-dialkyl side-chain substituted thiophene DPP end-capped with a phenyl group (Ph-TDPP-Ph) in FETs which were fabricated by vacuum deposition and solvent coating. Grazing incidence X-ray diffraction (GIXRD) from bottom-gate, bottom-contact FET architectures were measured with and without biasing. Ph-TDPP-Ph reveals polymorphic structure with π-conjugated stacking direction oriented in-plane. The unit cell comprises either one monomer with a=20.89 Å, b=13.02 Å, c=5.85 Å, α=101.4°, β=90.6°, and γ=94.7° for one phase (TR1), or two monomers with a=24.92 Å, b=25.59 Å, c=5.42 Å, α=80.3°, β=83.5°, and γ=111.8° for the second phase (TR2). The TR2 phase thus signals a shift from a coplanar to herringbone orientation of the molecules. The device performance is sensitive to the ratio of the two triclinic phases found in the film. Some of the best FET performances with p-type carrier mobilities of 0.1 cm2/Vs and on/off ratio of 106 are for films that comprise mainly the TR1 phase. GIXRD from in-operando FETs demonstrates the crystalline stability of Ph-TDPP-Ph.

General information
State: Accepted/In press
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, University of Missouri, Technical University of Denmark, Indian Institute of Science Bangalore, University of Warwick, University of Southern Denmark
Authors: Pickett, A. (Ekstern), Torkkeli, M. (Intern), Mukhopadhyay, T. (Ekstern), Puttaraju, B. (Ekstern), Laudari, A. (Ekstern), Lauritzen, A. (Ekstern), Bikondoa, O. (Ekstern), Kjelstrup-Hansen, J. (Ekstern), Knaapila, M. (Intern), Patil, S. (Ekstern), Guha, S. (Ekstern)
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Damping properties of non-conductive composite materials for applications in power transmission pylons

This study aims to characterize the fibre direction dependent damping properties of non-conductive composite materials to be used in newly designed electrical power transmission pylons, on which the conducting cables will be directly connected. Thus, the composite structure can be designed both to insulate and to act as a damper to avoid for example conductor line galloping. In order to predict the damping of the composite materials, a comprehensive analysis on a representative unidirectional laminate was carried out. The fibre direction dependent damping analysis of glass andaramid reinforced epoxy and vinylester, partly reinforced with nanoclay or fibre-hybridized, was investigated using a Dynamic Mechanical Thermal Analysis and a Vibrating Beam Testing procedure for five different fibre orientations (0°, 30°, 45°, 60° and 90°). The focus was on damping behaviour evaluation at low temperatures (-20°C and 0°C) and low vibration frequencies (0.5 Hz, 1 Hz and 2 Hz), in order to represent the environmental conditions of vibrating conductor lines during. The prediction of the damping behaviour for coupon-level specimens with three balanced laminates was successfully carried out with a maximal deviation of maximal 12.1%.

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Organisations: Department of Mechanical Engineering, Solid Mechanics, Department of Physics, Neutrons and X-rays for Materials Physics, Hochschule für Technik
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Scopus rating (2017): SNIP 0.898 SJR 0.555 CiteScore 1.57
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Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.573 SNIP 0.876 CiteScore 1.4
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.612 SNIP 1.188 CiteScore 1.44
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Decomposing the Bragg glass and the peak effect in a Type-II superconductor

Adding impurities or defects destroys crystalline order. Occasionally, however, extraordinary behaviour emerges that cannot be explained by perturbing the ordered state. One example is the Kondo effect, where magnetic impurities in metals drastically alter the temperature dependence of resistivity. In Type-II superconductors, disorder generally works to pin vortices, giving zero resistivity below a critical current $j_c$. However, peaks have been observed in the temperature and field dependences of $j_c$. This peak effect is difficult to explain in terms of an ordered Abrikosov vortex lattice. Here we test the widespread paradigm that an order-disorder transition of the vortex ensemble drives the peak effect. Using neutron scattering to probe the vortex order in superconducting vanadium, we uncover an order-disorder transition from a quasi-long-range-ordered phase to a vortex glass. The peak effect, however, is found to lie at higher fields and temperatures, in a region where thermal fluctuations of individual vortices become significant.

General information

State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Department of Wind Energy, Wind Turbine Structures and Component Design, University of Fribourg, Institut Laue-Langevin, University of Birmingham
Authors: Toft-Petersen, R. (Intern), Abrahamsen, A. B. (Intern), Balog, S. (Ekstern), Porcar, L. (Ekstern), Laver, M. (Ekstern)
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Journal: Nature Communications
Computer-based materials design plays an essential role in the development of new materials. Accurate prediction of the materials behavior during manufacturing and applications relies on accurate and complete materials databases. Traditional ways of material parameters measurements typically use idealized samples and sample environments, which may not be representative of the engineering processing and real-life usage. Moreover, material parameters are typically measured one at a time; thus it is time-consuming and costly to measure material parameters with large spectrum. In this thesis, a fitting methodology is proposed to determine material parameters by comparison between 4D x-ray experiments and phase-field simulations. The evolution of material microstructures is measured at a condition that mimics realistic engineering manufacturing and applications with 3D non-destructive in situ x-ray techniques. Starting from one snapshot of the experimental microstructure, the evolution of the 3D material microstructure is simulated using a phase-field model. An iterative optimization technique is used to find the values of material parameters that yield the best match between the simulated microstructure and the measured microstructure in a global manner. The proposed method is demonstrated on a simple case to fit two material parameters: the liquid diffusion coefficient and the capillary length of a hypoeutectic Al-Cu alloy, and a complicated case to fit hundreds of material parameters: the reduced grain boundary mobilities of pure iron. Results show that the proposed method is capable of providing reliable measurements of material parameters that are difficult to measure in traditional ways and can determine many - possibly all relevant - values of material parameters simultaneously. Moreover, the method developed is broadly applicable to many materials systems and experiments that provide 3D microstructure evolution.
Determination of the fibre orientation distribution of a mineral wool network and prediction of its transverse stiffness using X-ray tomography

A method to determine the orientation and diameter distributions of mineral wool fibre networks using X-ray tomography and image analysis is presented. The method is applied to two different types of mineral wool: glass wool and stone wool. The orientation information is obtained from the computation of the structure tensor, and the diameter is estimated by applying a greyscale granulometry. The results of the image analysis indicate the two types of fibres are distributed in a 2D planar arrangement with the glass wool fibres showing a higher degree of planarity than the stone wool fibres. The orientation information is included in an analytical model based on an Euler–Bernoulli beam approximation. The model enables prediction of the transverse stiffness. It is indicated that the glass wool transverse stiffness is lower than the stone wool transverse stiffness. Comparison with experimental results confirms the assumption that the underlying deformation mechanism of mineral wool is the bending of fibre segments between bonds.

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Organisations: Department of Wind Energy, Composites and Materials Mechanics, Department of Physics, Neutrons and X-rays for Materials Physics, Rockwool International, Xnovo Technology ApS
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BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.49 SJR 0.769 SNIP 1.072
Web of Science (2016): Indexed yes
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Scopus rating (2015): SJR 0.792 SNIP 1.059 CiteScore 2.36
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.963 SNIP 1.388 CiteScore 2.54
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.926 SNIP 1.451 CiteScore 2.36
Deterministic phase measurements exhibiting super-sensitivity and super-resolution

Phase super-sensitivity is obtained when the sensitivity in a phase measurement goes beyond the quantum shot noise limit, whereas super-resolution is obtained when the interference fringes in an interferometer are narrower than half the input wavelength. Here we show experimentally that these two features can be simultaneously achieved using a relatively simple setup based on Gaussian states and homodyne measurement. Using 430 photons shared between a coherent and a squeezed vacuum state, we demonstrate a 22-fold improvement in the phase resolution, while we observe a 1.7-fold improvement in the sensitivity. In contrast to previous demonstrations of super-resolution and super-sensitivity, this approach is fully deterministic.

General information
State: Published
Organisations: Department of Physics, Quantum Physics and Information Technology, Palacky University
Authors: Schäfermeier, C. (Intern), Ježek, M. (Ekstern), Madsen, L. S. (Intern), Gehring, T. (Intern), Andersen, U. L. (Intern)
Deuterium temperature, drift velocity, and density measurements in non-Maxwellian plasmas at ASDEX Upgrade

General information
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Organisations: Department of Physics, Plasma Physics and Fusion Energy, Max-Planck-Institut fur Plasmaphysik, University of Milano Bicocca
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Development of a Josephson vortex two-state system based on a confocal annular Josephson junction: Paper

We report theoretical and experimental work on the development of a Josephson vortex two-state system based on a confocal annular Josephson tunnel junction (CAJTJ). The key ingredient of this geometrical configuration is a periodically variable width that generates a spatial vortex potential with bistable states. This intrinsic vortex potential can be tuned by an externally applied magnetic field and tilted by a bias current. The two-state system is accurately modeled by a one-dimensional sine-Gordon like equation by means of which one can numerically calculate both the magnetic field needed to set the vortex in a given state as well as the vortex-depinning currents. Experimental data taken at on high-quality Nb/Al–AlOx/Nb CAJTJs with an individual trapped fluxon advocate the presence of a robust and finely tunable double-well potential for which reliable manipulation of the vortex state has been classically demonstrated. The vortex is prepared in a given potential by means of an externally applied magnetic field, while the state readout is accomplished by measuring the vortex-depinning current in a small magnetic field. Our proof of principle experiment convincingly demonstrates that the proposed vortex two-state system based on CAJTJs is robust and workable.
Directing a Non-Heme Iron(III)-Hydroperoxide Species on a Trifurcated Reactivity Pathway

The reactivity of \([\text{Fe}^{\text{III}}(\text{tpena})]^2+\) (tpena=N,N,N’-tris(2-pyridylmethyl)ethylenediamine-N’-acetate) as a catalyst for oxidation reactions depends on its ratio to the terminal oxidant \(\text{H}_2\text{O}_2\) and presence or absence of sacrificial substrates. The outcome can be switched between: 1) catalysed \(\text{H}_2\text{O}_2\) disproportionation, 2) selective catalytic oxidation of methanol or benzyl alcohol to the corresponding aldehyde, or 3) oxidative decomposition of the tpena ligand. A common mechanism is proposed involving homolytic O-O cleavage in the detected transient purple low-spin \((S=1/2)\) \([\text{tpenaH}][\text{Fe}^{\text{III}}\text{O-OH}]^2+\). The resultant iron(IV) oxo and hydroxyl radical both participate in controllable hydrogen-atom transfer (HAT) reactions. Consistent with the presence of a weaker σ-donor carboxylate ligand, the most pronounced difference in the spectroscopic properties of \([\text{Fe}(\text{OOH})(\text{tpenaH})]^+\) and its conjugate base, \([\text{Fe}(\text{OO})(\text{tpenaH})])^-\), compared to non-heme iron(III) peroxide analogues supported by neutral multidentate N-only ligands, are slightly blue-shifted maxima of the visible absorption band assigned to ligand-to-metal charge-transfer (LMCT) transitions and, corroborating this, lower Fe\(^{\text{III}}\)/Fe\(^{\text{II}}\) redox potentials for the pro-catalysts.

General information

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Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, University of Southern Denmark, University of Groningen
Authors: Wegeberg, C. (Ekstern), Lauritsen, F. R. (Ekstern), Frandsen, C. (Intern), Mørup, S. (Intern), Browne, W. R. (Ekstern), Mckenzie, C. J. (Ekstern)
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BFI (2014): BFI-level 2
Dissociation of two-dimensional excitons in monolayer WSe$_2$

Two-dimensional (2D) semiconducting materials are promising building blocks for optoelectronic applications, many of which require efficient dissociation of excitons into free electrons and holes. However, the strongly bound excitons arising from the enhanced Coulomb interaction in these monolayers suppresses the creation of free carriers. Here, we identify the main exciton dissociation mechanism through time and spectrally resolved photocurrent measurements in a monolayer WSe$_2$ p-n junction. We find that under static inplane electric field, excitons dissociate at a rate corresponding to the one predicted for tunnel ionization of 2D Wannier-Mott excitons. This study is essential for understanding the photoresponse of 2D semiconductors and offers design rules for the realization of efficient photodetectors, valley dependent optoelectronics, and novel quantum coherent phases.
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), Lăcătuşu, 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)

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BFI (2016): BFI-level 2

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Web of Science (2016): Indexed yes

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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

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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

Scopus rating (2008): SJR 6.194 SNIP 2.837

Web of Science (2008): Indexed yes

Scopus rating (2007): SJR 5.95 SNIP 2.738
Effect of porosity on the ferroelectric and piezoelectric properties of (Ba$_{0.85}$Ca$_{0.15}$)(Zr$_{0.1}$Ti$_{0.9}$)O$_3$ (BCZT) piezoelectric ceramics

The ferroelectric and piezoelectric properties of (Ba$_{0.85}$Ca$_{0.15}$)(Zr$_{0.1}$Ti$_{0.9}$)O$_3$ (BCZT) ceramics were measured as a function of porosity. Porous BCZT ceramics were fabricated using the sacrificial fugitive technique. Two different pore morphologies were induced by adding polymeric microspheres and fibres as the pore-forming agents. Increasing porosity led to decreasing ferroelectric and piezoelectric properties due to a reduction of polarisable BCZT ceramic available. With the benefit of being a lead-free piezoelectric material, porous BCZT ceramics may be considered for acoustic impedance matching in actuator and sensor applications, and also as a functional component in biomedical applications.
Effects of Zr Doping on Magnetic and Structural Properties of DyBa$_2$Cu$_3$O$_{7-δ}$ Thin Films

DyBa$_2$(Cu$_{1-x}$Zr$_x$)$_3$O$_{7-δ}$ thin films (with $x = 0.00, 0.02, 0.04,$ and $0.06$) were synthesized using the chemical solution deposition method on single crystalline LaAlO$_3$ 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 DyBa$_2$(Cu$_{1-x}$Zr$_x$)$_3$O$_{7-δ}$ thin films, with only minor reflections due to the presence of Dy$_2$O$_3$ and BaZrO$_3$ phases. Narrow...
transitions with $\Delta T_c$ 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 $J_c$ 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 $J_c$ value ($J_c = 3.5$ MA/cm$^2$, 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 ($F_p$ versus $B$) reveal a significant improvement over the magnetic field range investigated of the maximum pinning force for Zr-doped samples. We found $F_{Maxp} = 1.7$ GN/m$^3$ and 3.8 GN/m$^3$ 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)

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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
Electron–phonon interaction and transport properties of metallic bulk and monolayer transition metal dichalcogenide TaS$_2$

Transition metal dichalcogenides have recently emerged as promising two-dimensional materials with intriguing electronic properties. Existing calculations of intrinsic phonon-limited electronic transport so far have concentrated on the semiconducting members of this family. In this paper we extend these studies by investigating the influence of electron–phonon coupling on the electronic transport properties and band renormalization of prototype inherent metallic bulk and monolayer TaS$_2$. Based on density functional perturbation theory and semi-classical Boltzmann transport calculations, promising room temperature mobilities and sheet conductances are found, which can compete with other established 2D materials, leaving TaS$_2$ as promising material candidate for transparent conductors or as atomically thin interconnects. Throughout the paper, the electronic and transport properties of TaS$_2$ are compared to those of its isoelectronic counterpart TaSe$_2$ and additional informations to the latter are given. We furthermore comment on the conventional superconductivity in TaS$_2$, where no phonon-mediated enhancement of $T_C$ in the monolayer compared to the bulk state was found.

**General information**

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Authors: Hinsche, N. F. (Intern), Thygesen, K. S. (Intern)  
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Web of Science (2017): Indexed yes  
BFI (2016): BFI-level 1  
Scopus rating (2016): CiteScore 4.26 SJR 2.314 SNIP 0.915  
Web of Science (2016): Indexed yes  
BFI (2015): BFI-level 1  
Scopus rating (2015): SJR 4.602 SNIP 1.009 CiteScore 5.89
Electroreduction of CO on Polycrystalline Copper at Low Overpotentials

Cuis the only monometallic electrocatalyst to produce highly reduced products from CO₂ selectively because of its intermediate binding of CO. We investigate the performance of polycrystalline Cu for the electroreduction of CO in alkaline media (0.1 M KOH) at low overpotentials (−0.4 to −0.6 V vs RHE). We find that polycrystalline Cu is highly active at these potentials. The overall CO reduction rates are comparable to those of the nanostructured forms of the material, albeit with a distinct product distribution. While nanostructured forms of Cu favor alcohols, polycrystalline Cu produces greater amounts of C₂ and C₃ aldehydes, as well as ethylene.

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Main Research Area: Technical/natural sciences

Electrocathodic Reduction of CO in Alkaline Media using a Copper-Platinum(111) Alloy

The relationship between the binding of the reaction intermediates and oxygen reduction activity in alkaline media was experimentally explored. By introducing Cu into the 2nd surface layer of a Pt(111) single crystal, the surface reactivity was tuned. In both 0.1 m NaOH and 0.1 m KOH, the optimal catalyst should exhibit OH binding circa 0.1 eV weaker than Pt(111), via a Sabatier volcano; this observation suggests that the reaction is mediated via the same surface bound intermediates as in acid, in contrast to previous reports. In 0.1 m KOH, the alloy catalyst at the peak of the volcano exhibits a maximum activity of 101±8 mA cm⁻² at 0.9 V vs. a reversible hydrogen electrode (RHE). This activity constitutes a circa 60-fold increase over Pt(111) in 0.1 m HClO₄.

General information
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Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics, University of Copenhagen, Technische Universität München, Ruhr University Bochum
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Elucidation of the Oxygen Reduction Volcano in Alkaline Media using a Copper-Platinum(111) Alloy

The relationship between the binding of the reaction intermediates and oxygen reduction activity in alkaline media was experimentally explored. By introducing Cu into the 2nd surface layer of a Pt(111) single crystal, the surface reactivity was tuned. In both 0.1(M) NaOH and 0.1(M) KOH, the optimal catalyst should exhibit OH binding circa 0.1 eV weaker than Pt(111), via a Sabatier volcano; this observation suggests that the reaction is mediated via the same surface bound intermediates as in acid, in contrast to previous reports. In 0.1(M) KOH, the alloy catalyst at the peak of the volcano exhibits a maximum activity of 10 ± 8 mAcm² at 0.9 V vs. a reversible hydrogen electrode (RHE). This activity constitutes a circa 60-fold increase over Pt(111) in 0.1(M) HClO₄.
Enabling real-time detection of electrochemical desorption phenomena with sub-monolayer sensitivity

Electrochemical reactions play an increasingly important role in sustainable energy conversion and chemical synthesis. Better understanding of catalytic mechanisms at electrode surfaces is thus important for the transition to a clean-energy economy, but is hindered by the difficulty of real-time detection of reaction products and intermediates during electrochemistry experiments. Herein, we present a new type of electrochemistry mass spectrometry (EC-MS) based on a versatile gas inlet to vacuum fabricated onto a silicon microchip, and compare it to established techniques with focus on sensitivity, time response, and mass transport. The inlet system is able to capture reactant molecules directly from an electrode surface and pass them on to a mass spectrometer on a sub-second time scale with 100% collection efficiency for quantitative analysis with unprecedented sensitivity. The high sensitivity and fast time-response, coupled with well-characterized mass transport of both reactants and products in this setup enables sub-turnover resolution for analysis of electrochemical reactions. The technology and concepts presented here can serve as a platform to improve in-situ mass spectrometry in electrochemistry as well as other fields.

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Engineering Ni-Mo-S Nanoparticles for Hydrodesulfurization

Nanoparticle engineering for catalytic applications requires both a synthesis technique for the production of well-defined nanoparticles and measurements of their catalytic performance. In this paper, we present a new approach to rationally engineering highly active Ni-Mo-S nanoparticle catalysts for hydrodesulfurization (HDS), i.e., the removal of sulfur from fossil fuels. Nanoparticle catalysts are synthesized by the sputtering of a Mo_{75}Ni_{25} metal target in a reactive atmosphere of Ar and H_{2}S followed by the gas aggregation of the sputtered material into nanoparticles. The nanoparticles are filtered by a quadrupole mass filter and subsequently deposited on a planar substrate, such as a grid for electron microscopy or a microreactor. By varying the mass of the deposited nanoparticles, it is demonstrated that the Ni-Mo-S nanoparticles can be tuned into fullerene-like particles, flat-lying platelets, and upright-oriented platelets. The nanoparticle morphologies provide different abundances of Ni-Mo-S edge sites, which are commonly considered the catalytically important sites. Using a microreactor system, we assess the catalytic activity of the Ni-Mo-S nanoparticles for the HDS of dibenzothiophene. The measurements show that platelets are twice as active as the fullerene-like particles, demonstrating that the Ni-Mo-S edges are more active than basal planes for the HDS. Furthermore, the upright-standing orientation of platelets show an activity that is six times higher than the fullerene-like particles, demonstrating the importance of the edge site number and accessibility to reducing, e.g., sterical hindrance for the reacting molecules.

General information
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Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics, Haldor Topsoe AS
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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
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BFI (2009): BFI-level 2
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
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Organisations: Department of Applied Mathematics and Computer Science, Department of Physics, Plasma Physics and Fusion Energy, Dynamical Systems, Bogolyubov Institute for Theoretical Physics Nasu
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Main Research Area: Technical/natural sciences
Examining the rudimentary steps of the oxygen reduction reaction on single-atomic Pt using Ti-based non-oxide supports

In the attempt to reduce the high-cost and improve the overall durability of Pt-based electrocatalysts for the oxygen reduction reaction (ORR), density-functional theory (DFT) calculations have been performed to study the energetics of the elementary steps that occur during ORR on TiN(100)- and TiC(100)-supported single Pt atoms. The O₂ and OOH* dissociation processes on Pt/TiN(100) are determined to be non-activated (i.e. "barrier-less" dissociation) while an activation energy barrier of 0.19 and 0.51eV is found for these dissociation processes on Pt/TiC(100), respectively. Moreover, the series pathway (which is characterized by the stable OOH* molecular intermediate) on Pt/TiC(100) is predicted to be more favorable than the direct pathway. Our electronic structure analysis supports a strong synergistic cooperative effect by these non-oxide supports (TiN and TiC) on the reduced state of the single-atom Pt catalyst, and directly influences the rudimentary ORR steps on these single-atom platinized supports.

General information
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Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics, Yonsei University, Korea Advanced Institute of Science and Technology, Chungbuk National University
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Scopus rating (2016): CiteScore 4.3 SJR 1.148 SNIP 1.494
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Scopus rating (2015): SJR 0.931 SNIP 1.414 CiteScore 3.74
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Scopus rating (2014): SJR 0.865 SNIP 1.445 CiteScore 3.25
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.691 SNIP 1.118 CiteScore 2.19
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.795 SNIP 1.299 CiteScore 2.31
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Scopus rating (2011): SJR 0.85 SNIP 1.176 CiteScore 2.25
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Scopus rating (2010): SJR 0.838 SNIP 1.026
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.707 SNIP 1.049
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Scopus rating (2008): SJR 0.494 SNIP 0.77
Scopus rating (2007): SJR 0.469 SNIP 0.985
Scopus rating (2006): SJR 0.341 SNIP 0.599
Scopus rating (2005): SJR 0.474 SNIP 0.933
Scopus rating (2004): SJR 0.507 SNIP 1.057
Scopus rating (2003): SJR 0.373 SNIP 0.736
Scopus rating (2002): SJR 0.38 SNIP 1.064
Scopus rating (2001): SJR 0.31 SNIP 0.583
Exploration versus Exploitation in Global Atomistic Structure Optimization

The ability to navigate vast energy landscapes of molecules, clusters, and solids is a necessity for discovering novel compounds in computational chemistry and materials science. For high-dimensional systems, it is only computationally feasible to search a small portion of the landscape, and hence, the search strategy is of critical importance. Introducing Bayesian optimization concepts in an evolutionary algorithm framework, we quantify the concepts of exploration and exploitation in global minimum searches. The method allows us to control the balance between probing unknown regions of the landscape (exploration) and investigating further regions of the landscape known to have low-energy structures (exploitation). The search for global minima structures proves significantly faster with the optimal balance for three test systems (molecular compounds) and to a lesser extent also for a crystalline surface reconstruction. In addition, global search behaviors are analyzed to provide reasonable grounds for an optimal balance for different problems.
Feasibility and resolution limits of opto-magnetic imaging of neural network activity in brain slices using color centers in diamond

We suggest a novel approach for wide-field imaging of the neural network dynamics of brain slices that uses highly sensitivity magnetometry based on nitrogen-vacancy (NV) centers in diamond. Invitro recordings in brain slices is a proven method for the characterization of electrical neural activity and has strongly contributed to our understanding of the mechanisms that govern neural information processing. However, this traditional approach only acquires signals from a few positions, which severely limits its ability to characterize the dynamics of the underlying neural networks. We suggest to extend its scope using NV magnetometry-based imaging of the neural magnetic fields across the slice. Employing comprehensive computational simulations and theoretical analyses, we determine the spatiotemporal characteristics of the neural fields and the required key performance parameters of an NV magnetometry-based imaging setup. We investigate how the technical parameters determine the achievable spatial resolution for an optimal 2D reconstruction of neural currents from the measured field distributions. Finally, we compare the imaging of neural slice activity with that of a single planar pyramidal cell. Our results suggest that imaging of slice activity will be possible with the upcoming generation of NV magnetic field sensors, while single-shot imaging of planar cell activity remains challenging.
Fundamental limitation of electrocatalytic methane conversion to methanol
The electrochemical oxidation of methane to methanol at remote oil fields where methane is flared is the ultimate solution to harness this valuable energy resource. In this study we identify a fundamental surface catalytic limitation of this process in terms of a compromise between selectivity and activity, as oxygen evolution is a competing reaction. By investigating two classes of materials, rutile oxides and two-dimensional transition metal nitrides and carbides (MXenes), we find a linear relationship between the energy needed to activate methane, i.e. to break the first C-H bond, and oxygen binding energies on the surface. Based on a simple kinetic model we can conclude that in order to obtain sufficient activity oxygen has to bind weakly to the surface but there is an upper limit to retain selectivity. Few potentially interesting candidates are found but this relatively simple description enables future large scale screening studies for more optimal candidates.

General information
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Scopus rating (2017): CiteScore 4.04 SJR 1.686 SNIP 1.089
Web of Science (2017): Indexed yes
Gram-Scale Synthesis of Highly Active and Durable Octahedral PtNi Nanoparticle Catalysts for Proton Exchange Membrane Fuel Cell

Proton exchange membrane fuel cells (PEMFC) are regarded as a promising renewable energy source for a future hydrogen energy society. However, highly active and durable catalysts are required for the PEMFCs because of their intrinsic high overpotential at the cathode and operation under the acidic condition for oxygen reduction reaction (ORR). Since the discovery of the exceptionally high surface activity of $\text{Pt}_3\text{Ni}(111)$, the octahedral PtNi nanoparticles have been synthesized and tested. Nonetheless, their milligram-scale synthesis method and poor durability make them unsuitable for the commercialization of PEMFCs. In this study, we focus on gram-scale synthesis of octahedral PtNi nanoparticles with Pt overlayers (PtNi@Pt) supported on the carbon, resulting in enhanced catalytic activity and durability. Such PtNi@Pt catalysts show high mass activity ($1.24 \text{ A mgPt}^{-1}$) at 0.9 V (vs RHE) for the ORR, compared to commercial Pt/C ($0.22 \text{ A mgPt}^{-1}$). Single-cell performance and electrochemical impedance spectroscopy (EIS) were also tested. The PtNi@Pt catalysts showed enhanced current density of $3.1 \text{ A cm}^{-2}$ at 0.6 V in O2 flow while the commercial Pt/C had the value of $2.5 \text{ A cm}^{-2}$. After 30,000 cycles of the accelerated degradation test (ADT), the PtNi@Pt still showed better performance than the commercial Pt/C in a single-cell system. The Pt layers deposition could enhance the catalytic performance and durability of octahedral PtNi nanoparticles.

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Scopus rating (2017): CiteScore 10.92 SJR 3.152 SNIP 2.359
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
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Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 2.326 SNIP 2.16 CiteScore 7.72
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.322 SNIP 2.206 CiteScore 6.92
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.391 SNIP 2.154 CiteScore 6.42
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 2.65 SNIP 2.234 CiteScore 6.08
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 2.606 SNIP 2.351 CiteScore 6.14
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Hall effect measurement for precise sheet resistance and thickness evaluation of Ruthenium thin films using non-equidistant four-point probes

We present a new micro Hall effect measurement method using non-equidistant electrodes. We show theoretically and verify experimentally that it is advantageous to use non-equidistant electrodes for samples with low Hall sheet resistance. We demonstrate the new method by experiments where Hall sheet carrier densities and Hall mobilities of Ruthenium thin films (3-30 nm) are determined. The measurements show that it is possible to measure Hall mobilities as low as 1 cm²V⁻¹s⁻¹ with a relative standard deviation of 2-3%. We show a linear relation between measured Hall sheet carrier density and film thickness. Thus, the method can be used to monitor thickness variations of ultra-thin metal films.

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Web of Science (2017): Indexed Yes
Scopus rating (2016): CiteScore 1.32 SJR 0.957 SNIP 0.715
Web of Science (2016): Indexed yes
Hierarchically porous, ultra-strong reduced graphene oxide-cellulose nanocrystal sponges for exceptional adsorption of water contaminants

Self-assembly of graphene oxide (GO) nanosheets into porous 3D sponges is a promising approach to exploit their capacity to adsorb contaminants while facilitating the recovery of the nanosheets from treated water. Yet, forming mechanically robust sponges with suitable adsorption properties presents a significant challenge. Ultra-strong and highly porous 3D sponges are formed using GO, vitamin C (VC), and cellulose nanocrystals (CNCs) - natural nanorods isolated from wood pulp. CNCs provide a robust scaffold for the partially reduced GO (rGO) nanosheets resulting in an exceptionally stiff nanohybrid. The concentration of VC as a reducing agent plays a critical role in tailoring the pore architecture of the sponges. By using excess amounts of VC, a unique hierarchical pore structure is achieved, where VC grains act as soft templates for forming millimeter-sized pores, the walls of which are also porous and comprised of micron-sized pores. The unique hierarchical pore structure ensures the interconnectivity of pores even at the core of large sponges as evidenced by micro and nano X-ray computed tomography. The unique pore architecture translates into an exceptional specific surface area for adsorption of a wide range of contaminants, such as dyes, heavy metals, pharmaceuticals and cyanotoxin from water.
Highly Durable Platinum Single-Atom Alloy Catalyst for Electrochemical Reactions

Single atomic Pt catalyst can offer efficient utilization of the expensive platinum and provide unique selectivity because it lacks ensemble sites. However, designing such a catalyst with high Pt loading and good durability is very challenging. Here, single atomic Pt catalyst supported on antimony-doped tin oxide (Pt1/ATO) is synthesized by conventional incipient wetness impregnation, with up to 8 wt% Pt. The single atomic Pt structure is confirmed by high-angle annular dark field scanning tunneling electron microscopy images and extended X-ray absorption fine structure analysis results. Density functional theory calculations show that replacing Sb sites with Pt atoms in the bulk phase or at the surface of SbSn or ATO is energetically favorable. The Pt1/ATO shows superior activity and durability for formic acid oxidation reaction, compared to a commercial Pt/C catalyst. The single atomic Pt structure is retained even after a harsh durability test, which is performed by repeating cyclic voltammetry in the range of 0.05–1.4 V for 1800 cycles. A full cell is fabricated for direct formic acid fuel cell using the Pt1/ATO as an anode catalyst, and an order of magnitude higher cell power is obtained compared to the Pt/C.
High pressure structural studies of conjugated molecules

This chapter highlights high pressure GPa level structural studies of conjugated polymers and their analogues: conjugated oligomers and molecules, and rigid rod polymers. Attention is placed on our recent studies of polyfluorenes.

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Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Bergische Universität Wuppertal, University of Missouri
Authors: Knaapila, M. (Intern), Torkkeli, M. (Intern), Scherf, U. (Ekstern), Guha, S. (Ekstern)
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High-Throughput Computational Assessment of Previously Synthesized Semiconductors for Photovoltaic and Photoelectrochemical Devices

Using computational screening we identify materials with potential use as light absorbers in photovoltaic or photoelectrochemical devices. The screening focuses on compounds of up to three different chemical elements which are abundant and nontoxic. A prescreening is carried out based on information from the Inorganic Crystal Structure Database and Open Quantum Materials Database. The light absorption, carrier mobility, defect tolerance, and stability of the materials are assessed by a set of simple computational descriptors. The identified 74 materials include a variety of...
pnictogenides, chalcogenides, and halides. Several recently investigated light absorbers, such as CsSnI3, CsSnBr3, and BaZrS3, appear on the list.

In-Situ XRD during Electrochemical CO Reduction on Cu
Almost all-successful CO2 and CO reduction catalysts to higher chain carbons are based on copper1, however various facets and pre-treatments of copper have shown to give a wide variety of product selectivity.2,3 Currently there are many unanswered questions regarding active sites and mechanisms thus fundamental studies are essential for this reaction. This talk will focus on in-situ monitoring the copper-copper oxide crystal structure at a variety of oxidative and reductive potentials. Using the synchrotron facilities at the SLAC national laboratory we were able to achieve an in-depth understand both of how deep the native oxide layer penetrates and how this oxide becomes reduced as we shift towards more cathodic potentials. This talk was also discuss under what conditions there is an amorphous copper oxide layer and what conditions lead to a crystalline copper oxide surface. This will be followed by a discussion of how the copper oxide effects the crystal structure of the metallic copper at the operating conditions.

Interlayer Excitons with Large Optical Amplitudes in Layered van der Waals Materials
Vertically stacked two-dimensional materials form an ideal platform for controlling and exploiting light-matter interactions at the nanoscale. As a unique feature, these materials host electronic excitations of both intra- and interlayer type with
distinctly different properties. In this Letter, using first-principles many-body calculations, we provide a detailed picture of the most prominent excitons in bilayer MoS2, a prototypical van der Waals material. By applying an electric field perpendicular to the bilayer, we explore the evolution of the excitonic states as the band alignment is varied from perfect line-up to staggered (Type II) alignment. For moderate field strengths, the lowest exciton has intralayer character and is almost independent of the electric field. However, we find higher lying excitons that have interlayer character. They can be described as linear combinations of the intralayer B exciton and optically dark charge transfer excitons, and interestingly, these mixed interlayer excitons have strong optical amplitude and can be easily tuned by the electric field. The first-principles results can be accurately reproduced by a simple excitonic model Hamiltonian that can be straightforwardly generalized to more complex van der Waals materials.
Electronic excitations in van der Waals heterostructures can have interlayer or intralayer character depending on the spatial localization of the involved charges (electrons and holes). In the case of neutral electron-hole pairs (excitons), both types of excitations have been explored theoretically and experimentally. In contrast, studies of charged trions have so far been limited to the intralayer type. Here we investigate the complete set of interlayer excitations in a MoS$_2$/WS$_2$ heterostructure using a novel ab initio method, which allows for a consistent treatment of both excitons and trions at the same theoretical footing. Our calculations predict the existence of bound interlayer trions below the neutral interlayer excitons. We obtain binding energies of 18/28 meV for the positive/negative interlayer trions with both electrons/holes located on the same layer. In contrast, a negligible binding energy is found for trions which have the two equally charged particles on different layers. Our results advance the understanding of electronic excitations in doped van der Waals heterostructures and their effect on the optical properties.
Internal Fiber Structure of a High-Performing, Additively Manufactured Injection Molding Insert

A standard mold is equipped with additively manufactured inserts in a rectangular shape produced with vat photo polymerization. While the lifetime compared to conventional materials such as brass, steel, and aluminum is reduced, the prototyping and design phase can be shortened significantly by using flexible and cost-effective additive manufacturing technologies. Higher production volumes still exceed the capability of additively manufactured inserts, which are overruled by the stronger performance of less-flexible but mechanically advanced materials. In this contribution, the internal structure of a high-performing, fiber-reinforced injection molding insert has been analyzed. The insert reached a statistically proven and reproducible lifetime of 4,500 shots, which significantly outperforms any other previously published additively manufactured inserts. Computer tomography, tensile tests and life cycle analysis have been performed in order to provide an understanding of the internal structure of the fiber-reinforced, additively manufactured injection molding inserts.

Layered Surface Detection for Virtual Unrolling

We present a method for virtual unrolling of a thin rolled object. From a volumetric image of the rolled object we obtain a flat image of the object’s surface, which allows visual inspection of the object and has a number of applications. Our method exploits the geometric constrains of the problem and detects a single rolled surface. For surface detection we adapt a solution to an optimal net surface problem, previously used for terrain-like and tubular surfaces. We present our approach on an example of a rolled sheet of
microelectronic, which has a layer of flexible polymer substrate and a thin metal layer lithographically coated onto the polymer. Our approach is automatic and robust. The unrolled image is undistorted, and the surface structures may be accurately quantified making our approach a good candidate for an industrial application of virtual unrolling.

Local Plasmon Engineering in Doped Graphene

Single-atom B or N substitutional doping in single-layer suspended graphene, realized by low-energy ion implantation, is shown to induce a dampening or enhancement of the characteristic interband $\pi$ plasmon of graphene through a high-resolution electron energy loss spectroscopy study using scanning transmission electron microscopy. A relative 16% decrease or 20% increase in the $\pi$ plasmon quality factor is attributed to the presence of a single substitutional B or N atom dopant, respectively. This modification is in both cases shown to be relatively localized, with data suggesting the plasmonic response tailoring can no longer be detected within experimental uncertainties beyond a distance of approximately 1 nm from the dopant. Ab initio calculations confirm the trends observed experimentally. Our results directly confirm the possibility of tailoring the plasmonic properties of graphene in the ultraviolet waveband at the atomic scale, a crucial step in the quest for utilizing graphene's properties toward the development of plasmonic and optoelectronic devices operating at ultraviolet frequencies.

General information
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Organisations: Department of Physics, Theoretical Atomic-scale Physics, Center for Nanostructured Graphene, SuperSTEM Laboratory, University of Leeds, Ömer Halisdemir University, Georg-August-Universität Göttingen, University of Limerick
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Web of Science (2017): Indexed yes
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Scopus rating (2016): CiteScore 13.65 SJR 6.948 SNIP 2.604
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
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BFI (2014): BFI-level 2
Low temperature bonding of heterogeneous materials using Al2O3 as an intermediate layer

Direct wafer bonding is a key enabling technology for many current and emerging photonic devices. Most prior work on direct wafer bonding has, however, focused on the Si platform for fabrication of silicon-on-insulator (SOI) and micro-electromechanical systems (MEMS). As a result, a universal bonding solution for heterogeneous material systems has not yet been developed. This has been a roadblock in the realization of novel devices which need the integration of new semiconductor platforms such as III-V on Si, Ge on Sapphire, LiNbO3 on GaAs etc. The large thermal expansion coefficient mismatch in the hetero-material systems limits the annealing to low temperatures to avoid stressed films. This work explores the use of Al2O3 as an intermediate layer for bonding heterogeneous materials. The key to achieve a stronger bond is to maximize the hydroxyl group density of the bonding interfaces. The use of Al2O3 helps achieve that, since it has a high hydroxyl group density (around 18 OH/nm² at RT) which is approximately 4 times that of a Si surface. This work optimizes the bonding process using Al2O3 by studying the contribution of Al2O3 deposition parameters. An optimized process is presented and applied to bond GaAs on Sapphire and InP on SiO2/Si.

General information

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Organisations: Department of Photonics Engineering, Nanophotonic Devices, Nanophotonics Theory and Signal Processing, High-Speed Optical Communication, Department of Physics, Neutrons and X-rays for Materials Physics, Experimental Surface and Nanomaterials Physics, Department of Micro- and Nanotechnology, Silicon Microtechnology, Centre of Excellence for Silicon Photonics for Optical Communications
Authors: Sahoo, H. K. (Intern), Ottaviano, L. (Intern), Zheng, Y. (Intern), Hansen, O. (Intern), Yvind, K. (Intern)
Number of pages: 7
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Main Research Area: Technical/natural sciences
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.
Magnetic and transport properties of conjugated and cumulated molecules: the π-system enlightens part of the story

We have investigated the intramolecular magnetic exchange coupling constants (J) for a series of nitronyl nitroxide diradicals connected by a range of linear conjugated and cumulene couplers focusing on the unusual π-interaction properties within the couplers. Distance between radical centers, spin density within the couplers, as well as the dihedral angles between the radical centers and the plane of the coupler influence the strength of magnetic coupling. We also establish that with the increase in the length of the coupler, the strength of magnetic interaction in conjugated and cumulene systems varies in a different way. Transport calculations show that with the increase in chain length, diradicals based on cumulene containing an even number of carbon atoms act as better conductors than cumulenes with an odd number of carbon atoms. It is also observed that with the increase in the length of the conjugated coupler based diradicals, transmission does not vary in a sequential way.

General information
State: Published
Organisations: Department of Physics, Theoretical Atomic-scale Physics, University of North Bengal
Authors: Sarbadhikary, P. (Ekstern), Shil, S. (Intern), Misra, A. (Ekstern)
Pages: 9364-9375
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Main Research Area: Technical/natural sciences
Magnetic ground state and magnon-phonon interaction in multiferroic h-YMnO₃

Inelastic neutron scattering has been used to study the magnetoelastic excitations in the multiferroic manganite hexagonal YMnO₃. An avoided crossing is found between magnon and phonon modes close to the Brillouin zone boundary in the (a,b) plane. Neutron polarization analysis reveals that this mode has mixed magnon-phonon character. An external magnetic field along the c axis is observed to cause a linear field-induced splitting of one of the spin-wave branches. A theoretical description is performed, using a Heisenberg model of localized spins, acoustic phonon modes, and a magnetoelastic coupling via the single-ion magnetostriction. The model quantitatively reproduces the dispersion and intensities of all modes in the full Brillouin zone, describes the observed magnon-phonon hybridized modes, and quantifies the magnetoelastic coupling. The combined information, including the field-induced magnon splitting, allows us to exclude several of the earlier proposed models and point to the correct magnetic ground state symmetry, and provides an effective dynamic model relevant for the multiferroic hexagonal manganites.
The magnetic phase diagram of the quaternary borocarbide TbNi$_2$B$_2$C is investigated by direct means and by studying magnetoelastically 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.
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BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
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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
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Source: FindIt
Source-ID: 2435639374
Publication: Research - peer-review › Journal article – Annual report year: 2018
Modeling the adsorption of sulfur containing molecules and their hydrodesulfurization intermediates on the Co-promoted MoS$_2$ catalyst by DFT

Achieving ultra-deep hydrodesulfurization means enabling removal of the last fractions of sulfur, contained in refractory molecules, from oil. Improving the state-of-the-art Co-promoted MoS$_2$ (CoMoS) catalyst or the development of novel catalysts is crucial for this. Improving CoMoS requires more insight in the way sulfur containing molecules interact with it. Herein, we model the adsorption of sulfur containing molecules on the S-edge, M-edge, corner and basal plane of CoMoS using density functional theory. The obtained adsorption configurations and energies point to a preference towards physisorption at the S-edge and chemisorption in vacancies at the M-edge and corner. Smaller molecules, such as thiophene and methyldithiol, were found to prefer vacancies when adsorbing while larger, sterically hindered molecules as 4,6-dimethyldibenzothiophene prefer physisorption on the brim of the edges or the basal plane through van der Waals interactions. Hydrogenation generally leads to a preference towards adsorption at vacancies for thiophene and dibenzothiophene while for 4,6-dimethyldibenzothiophene hydrogenation leads to preferential adsorption on the S-edge brim, possibly explaining why 4,6-dimethyldibenzothiophene does not get desulfurized directly but follows a hydrogenation route. Thiolate formation energies were also calculated for the different molecules and used to predict which sites are most likely to be involved in breaking carbon-sulfur bonds. The thiolate formation energies show the inert nature of the basal plane towards breaking carbon-sulfur and sulfur-hydrogen bonds. Additionally, activation energies for thiophene and dibenzothiophene carbon-sulfur bond scission indicate that both molecules follow the direct desulfurization route on under-coordinated sites or vacancies.

General information
State: Published
Organisations: Department of Physics, University of Copenhagen, Haldor Topsoe AS
Authors: Šarić, M. (Intern), Rossmeisl, J. (Ekstern), Moses, P. G. (Ekstern)
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Scopus rating (2017): SNIP 1.85 SJR 2.397 CiteScore 6.99
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 7.27 SJR 2.451 SNIP 2.142
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 2.668 SNIP 2.177 CiteScore 7.23
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.688 SNIP 2.233 CiteScore 6.92
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.553 SNIP 2.091 CiteScore 6.42
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 3.006 SNIP 2.257 CiteScore 6.17
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 3.092 SNIP 2.214 CiteScore 6.23
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
Molecular scale structure and dynamics at an ionic liquid/electrode interface

After a century of research, the potential-dependent ion distribution at electrode/electrolyte interfaces is still under debate. In particular for solvent-free electrolytes such as room-temperature ionic liquids, classical theories for the electrical double layer are not applicable. Using a combination of in situ high-energy X-ray reflectivity and impedance spectroscopy measurements, we determined this distribution with sub-molecular resolution. We find oscillatory charge density profiles consisting of alternating anion- and cation-enriched layers at both cathodic and anodic potentials. This structure is shown to arise from the same ion-ion correlations dominating the liquid bulk structure. The relaxation dynamics of the interfacial structure upon charging/discharging were studied by impedance spectroscopy and time resolved X-ray reflectivity experiments with sub-millisecond resolution. The analysis revealed three relaxation processes of vastly different characteristic time scales: a 2 ms scale interface-normal ion transport, a 100 ms scale molecular reorientation, and a minute scale lateral ordering within the first layer.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Max Planck Institute for Polymer Research, Bar-Ilan University, European Synchrotron Radiation Facility
Authors: Reichert, P. (Ekstern), Kjær, K. S. (Intern), Brandt van Driel, T. (Intern), Mars, J. (Ekstern), Ochsmann, J. W. (Ekstern), Pontoni, D. (Ekstern), Deutsch, M. (Ekstern), Nielsen, M. M. (Intern), Mezger, M. (Ekstern)
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Journal: Faraday Discussions
Multi-q Mesoscale Magnetism in CeAuSb2

We report the discovery of a field driven transition from a single-q to multi-q spin density wave (SDW) in the tetragonal heavy fermion compound CeAuSb2. Polarized along c, the sinusoidal SDW amplitude is $1.8(2)$μB/Ce for $T \ll T_N = 6.25(10)$ K with a wave vector $q_1 = (\eta; \eta; 1/2)$ [3]. For $H \parallel c$, harmonics appearing at $2q_1$ evidence a striped magnetic texture below $\mu B H_1 = 2.78(1)$ T. Above $H_1$, these are replaced by coupled harmonics at $q_1 + q_2 = (2\eta; 0; 0)$ and $\mu B H_2 = 5.42(5)$ T, where satellites vanish and magnetization nonlinearly approaches saturation at $1.64(2)$μB/Ce for $\mu B H = 7$ T.

General information
State: Published
Organisations: Department of Physics, Johns Hopkins University, University of California at Irvine, University of Maryland, Paul Scherrer Institut
Authors: Marcus, G. G. (Ekstern), Kim, D. (Ekstern), Tutmaher, J. A. (Ekstern), Rodriguez-Rivera, J. A. (Ekstern), Birk, J. O. (Intern), Niedermeyer, C. (Ekstern), Lee, H. (Ekstern), Fisk, Z. (Ekstern), Broholm, C. L. (Ekstern)
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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
Mutual information of optical communication in phase-conjugating Gaussian channels
In all practical communication channels, the code word consists of Gaussian states and the measurement strategy is often a Gaussian detector such as homodyning or heterodyning. We investigate the communication performance using a phase-conjugated alphabet and joint Gaussian detection in a phase-insensitive amplifying channel. We find that a communication scheme consisting of a phase-conjugating alphabet of coherent states and a joint detection strategy significantly outperforms a standard coherent-state strategy based in individual detection. Moreover, we show that the performance can be further enhanced by using entanglement and that the performance is completely independent of the gain of the phase-insensitively amplifying channel.

General information
State: Published
Organisations: Department of Physics, Quantum Physics and Information Technology
Authors: Schafermeier, C. (Intern), Andersen, U. L. (Intern)
Number of pages: 5
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Volume: 97
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 0.886 SJR 1.288 CiteScore 2.46
Web of Science (2017): Indexed yes
Scopus rating (2016): CiteScore 2.25 SJR 1.482 SNIP 0.985
Nitrogen-vacancy ensemble magnetometry based on pump absorption

We demonstrate magnetic-field sensing using an ensemble of nitrogen-vacancy centers by recording the variation in the pump-light absorption due to the spin-polarization dependence of the total ground-state population. Using a 532 nm pump laser, we measure the absorption of native nitrogen-vacancy centers in a chemical-vapor-deposited diamond placed in a resonant optical cavity. For a laser pump power of 0.4 W and a cavity finesse of 45, we obtain a noise floor of ∼100 nT/√Hz spanning a bandwidth up to 125 Hz. We project a photon shot-noise-limited sensitivity of ∼1 pT/√Hz by optimizing the nitrogen-vacancy concentration and the detection method.
On the interpretation of Mössbauer spectra of magnetic nanoparticles

Mössbauer spectra of magnetic nanoparticles are usually influenced by fluctuations of the direction of the magnetic hyperfine field. In samples of non-interacting particles, the superparamagnetic relaxation usually results in spectra consisting of a sum of a sextet and a doublet with a temperature dependent area ratio. This is in accordance with the exponential dependence of the superparamagnetic relaxation time on particle size and temperature in combination with the particle size distribution. An alternative interpretation of these features is a first order magnetic transition from a magnetically ordered state to a paramagnetic state. We point out that this interpretation seems not to be correct, because the doublet component has been found to transform to a magnetically split component when relatively small magnetic fields are applied, and therefore it cannot be due to a paramagnetic state. In other cases, spectra of magnetic nanoparticles consist of sextets with asymmetrically broadened lines without the presence of doublets. It has been suggested that such spectra can be explained by a multilevel model, according to which relaxation takes place between a large number of states. We point out that spectra with asymmetrically broadened lines at least in some cases rather should be explained by the influence of magnetic inter-particle interactions on the magnetic fluctuations.

General information
State: Published
Organisations: Department of Micro- and Nanotechnology, Magnetic Systems, Department of Physics, Neutrons and X-rays for Materials Physics
Authors: Fock, J. (Intern), Hansen, M. F. (Intern), Frandsen, C. (Intern), Mørup, S. (Intern)
Pages: 11-21
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Main Research Area: Technical/natural sciences

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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
Herein we present surface sensitive operando XAS L-edge measurements on IrOx/RuO2 thin films as well as mass-selected RuOx and Ru nanoparticles. We observed shifts of the white line XAS peak toward higher energies with applied electrochemical potential. Apart from the case of the metallic Ru nanoparticles, the observed potential dependencies were purely core-level shifts caused by a change in oxidation state, which indicates no structural changes. These findings can be explained by different binding energies of oxygenated species on the surface of IrOx and RuOx. Simulated XAS spectra show that the average Ir oxidation state change is strongly affected by the coverage of atomic O. The observed shifts in oxidation state suggest that the surface has a high coverage of O at potentials just below the potential where oxygen evolution is exergonic in free energy. This observation is consistent with the notion that the metal-oxygen bond is stronger than ideal.
Phase-and-amplitude recovery from a single phase-contrast image using partially spatially coherent x-ray radiation: Paper

A simple method of phase-and-amplitude extraction is derived that corrects for image blurring induced by partially spatially coherent incident illumination using only a single intensity image as input. The method is based on Fresnel diffraction theory for the case of high Fresnel number, merged with the space-frequency description formalism used to quantify partially coherent fields and assumes the object under study is composed of a single-material. A priori knowledge of the object's complex refractive index and information obtained by characterizing the spatial coherence of the source is required. The algorithm was applied to propagation-based phase-contrast data measured with a laboratory-based micro-focus x-ray source. The blurring due to the finite spatial extent of the source is embedded within the algorithm as a simple correction term to the so-called Paganin algorithm and is also numerically stable in the presence of noise.
Phloem physics: mechanisms, constraints, and perspectives

Plants have evolved specialized vascular tissues for the distribution of energy, water, nutrients, and for communication. The phloem transports sugars from photosynthetic source regions (e.g. mature leaves) to sugar sinks (e.g. developing tissues such as buds, flowers, roots). Moreover, chemical signals such as hormones, RNAs and proteins also move in the phloem. Basic physical processes strongly limit phloem anatomy and function. This paper provides an overview of recent research and perspectives on phloem biomechanics and the physical constraints relevant to sugar transport in plants.

General information
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Organisations: Department of Physics, Biophysics and Fluids
Authors: Jensen, K. H. (Intern)
Number of pages: 5
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Web of Science (2018): Indexed yes
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Scopus rating (2017): SNIP 1.771 SJR 4.382 CiteScore 7.25
Web of Science (2017): Indexed Yes
Plasma particle sources due to interactions with neutrals in a turbulent scrape-off layer of a toroidally confined plasma

The conditions in the edge and scrape-off layer (SOL) of magnetically confined plasmas determine the overall performance of the device, and it is of great importance to study and understand the mechanics that drive transport in those regions. If a significant amount of neutral molecules and atoms is present in the edge and SOL regions, those will influence the plasma parameters and thus the plasma confinement. In this paper, it is displayed how neutrals, described by a fluid model, introduce source terms in a plasma drift-fluid model due to inelastic collisions. The resulting source terms are included in a four-field drift fluid model, and it is shown how an increasing neutral particle density in the edge and SOL regions influences the plasma particle transport across the lastclosed-flux-surface. It is found that an appropriate gas puffing rate allows for the edge density in the simulation to be self-consistently maintained due to ionization of neutrals in the confined region.

General information
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Organisations: Department of Physics, Plasma Physics and Fusion Energy, Theoretical Atomic-scale Physics
Authors: Thrysøe, A. S. (Intern), Løiten, M. (Intern), Madsen, J. (Intern), Naulin, V. (Intern), Nielsen, A. H. (Intern), Rasmussen, J. J. (Intern)
Number of pages: 9
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information
Journal: Physics of Plasmas
Volume: 25
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Article number: 032307
Porosity and density measurements of sodium acetate trihydrate for thermal energy storage

Sodium acetate trihydrate (SAT) can be used as phase change material in latent heat storage with or without utilizing supercooling. The change of density between liquid to solid state leads to formation of cavities inside the bulk SAT during solidification. Samples of SAT which had solidified from supercooled state at ambient temperature and samples which had solidified with a minimal degree supercooled were investigated. The temperature dependent densities of liquid and the two types of solid SAT were measured with a density meter and a thermomechanical analyzer. The cavities formed inside samples of solid SAT, which had solidified after a high or minimal degree of supercooling, were investigated by X-ray scanning and computer tomography. The apparent density of solid SAT depended on whether it solidified from a supercooled state or not. A sample which solidified from a supercooled liquid contained 15% cavities and had a density of 1.26 g/cm³ at 25 °C. SAT which had solidified with minimal supercooling contained 9% cavities and had a density of 1.34 g/cm³ at 25 °C. The apparent densities of the solid SAT samples were significant lower than the value of solid SAT reported in literature of 1.45 g/cm³. The density of liquid and supercooled SAT with extra water was also determined at different temperatures.

General information
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Organisations: Department of Civil Engineering, Section for Building Energy, Department of Physics, Neutrons and X-rays for Materials Physics, Department of Applied Mathematics and Computer Science, Image Analysis & Computer Graphics, University of Zaragoza, Technical University of Denmark, Graz University of Technology
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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
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Sodium acetate trihydrate, Density, Phase change material, X-ray tomography, Thermal energy storage, Cavity

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Publication: Research - peer-review › Journal article – Annual report year: 2018

Power to fuels and chemicals innovation challenge

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Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics, Stanford University, Haldor Topsoe AS, Stanford University
Authors: Kibsgaard, J. (Intern), Vesborg, P. C. K. (Intern), Chorkendorff, I. (Intern), Jaramillo, T. F. (Ekstern), Nørskov, J. K. (Ekstern), Moses, P. G. (Ekstern), Sehested, J. (Ekstern)
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Electronic versions:
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Pressure-induced transformations in Ce-Al metallic glasses: The role of stiffness of interatomic pairs
When high pressure is applied to Ce-Al metallic glasses, their disordered atomic structure exhibits some unusual properties like polyamorphism or transformation into a crystalline phase. In this work, we probe the atomic arrangement of Ce$_{55}$Al$_{45}$ and Ce$_{75}$Al$_{25}$ glasses by X-ray absorption spectroscopy and X-ray diffraction in the pressure range of 0–30 GPa. The pressure-dependent parameters of local environment of cerium atoms are evaluated by extended X-ray absorption fine structure (EXAFS) fitting. We demonstrate that due to compositional dependence of stiffness of Ce-Al pairs, densification of Ce$_{55}$Al$_{45}$ is accompanied by an increase of atomic size mismatch between Ce and Al stabilizing the
amorphous phase, while a decrease of the mismatch is observed in Ce$_{75}$Al$_{25}$ alloy which eventually leads to its devitrification at 25 GPa.
Projective measurement onto arbitrary superposition of weak coherent state bases

One of the peculiar features in quantum mechanics is that a superposition of macroscopically distinct states can exist. In optical system, this is highlighted by a superposition of coherent states (SCS), i.e. a superposition of classical states. Recently this highly nontrivial quantum state and its variant have been demonstrated experimentally. Here we demonstrate the superposition of coherent states in quantum measurement which is also a key concept in quantum mechanics. More precisely, we propose and implement a projection measurement onto an arbitrary superposition of two weak coherent states in optical system. The measurement operators are reconstructed experimentally by a novel quantum detector tomography protocol. Our device is realized by combining the displacement operation and photon counting, well established technologies, and thus has implications in various optical quantum information processing applications.
Prototype of the novel CAMEA concept—A backend for neutron spectrometers

General information
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Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Paul Scherrer Institut, University of Copenhagen, Ecole Polytechnique Federale de Lausanne (EPFL)
Authors: Markó, M. (Ekstern), Groitl, F. (Ekstern), Birk, J. O. (Ekstern), Freeman, P. G. (Ekstern), Lefmann, K. (Ekstern), Christensen, N. B. (Intern), Niedermayer, C. (Ekstern), Jurányi, F. (Ekstern), Lass, J. (Ekstern), Hansen, A. (Ekstern), Rennow, H. M. (Ekstern)
Number of pages: 13
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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
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.017 SNIP 1.277 CiteScore 1.45
Förster resonant energy transfer (FRET) measurements are widely used to obtain information about molecular interactions and conformations through the dependence of FRET efficiency on the proximity of donor and acceptor fluorophores. Fluorescence lifetime measurements can provide quantitative analysis of FRET efficiency and interacting population fraction. Many FRET experiments exploit the highly specific labelling of genetically expressed fluorescent proteins, applicable in live cells and organisms. Unfortunately, the typical assumption of fast randomization of fluorophore orientations in the analysis of fluorescence lifetime-based FRET readouts is not valid for fluorescent proteins due to their slow rotational mobility compared to their upper state lifetime. Here, previous analysis of effectively static isotropic distributions of fluorophore dipoles on FRET measurements is incorporated into new software for fitting donor emission decay profiles. Calculated FRET parameters, including molar population fractions, are compared for the analysis of simulated and experimental FRET data under the assumption of static and dynamic fluorophores and the intermediate regimes between fully dynamic and static fluorophores, and mixtures within FRET pairs, is explored. Finally, a method to correct the artefact resulting from fitting the emission from static FRET pairs with isotropic angular distributions to the (incorrect) typically assumed dynamic FRET decay model is presented.
Reduced sintering of mass-selected Au clusters on SiO₂ by alloying with Ti: an aberration-corrected STEM and computational study

Au nanoparticles represent the most remarkable example of a size effect in heterogeneous catalysis. However, a major issue hindering the use of Au nanoparticles in technological applications is their rapid sintering. We explore the potential of stabilizing Au nanoclusters on SiO₂ by alloying them with a reactive metal, Ti. Mass-selected Au/Ti clusters (400 000 amu) and Au₂057 clusters (405 229 amu) were produced with a magnetron sputtering, gas condensation cluster beam source in conjunction with a lateral time-of-flight mass filter, deposited onto a silica support and characterised by XPS and LEIS. The sintering dynamics of mass-selected Au and Au/Ti alloy nanoclusters were investigated in real space and real time with atomic resolution aberration-corrected HAADF-STEM imaging, supported by model DFT calculations. A strong anchoring effect was revealed in the case of the Au/Ti clusters, because of a much increased local interaction with the support (by a factor 5 in the simulations), which strongly inhibits sintering, especially when the clusters are more than ~0.60 nm apart. Heating the clusters at 100 °C for 1 h in a mixture of O₂ and CO, to simulate CO oxidation conditions, led to some
segregation in the Au/Ti clusters, but in line with the model computational investigation, Au atoms were still present on the surface. Thus size-selected, deposited nanoalloy Au/Ti clusters appear to be promising candidates for sustainable gold-based nanocatalysis.

**General information**

State: Published

Organisations: Experimental Surface and Nanomaterials Physics, Department of Physics, Università degli Studi di Milano-Bicocca, Swansea University, University of Birmingham

Authors: Niu, Y. (Ekster), Schlexer, P. (Ekster), Sebók, B. (Intern), Chorkendorff, I. (Intern), Pacchioni, G. (Ekster), Palmer, R. E. (Ekster)

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BFI (2017): BFI-level 2

Scopus rating (2017): SJR 2.934 SNIP 1.442 CiteScore 7.57

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

Web of Science (2012): Indexed yes

Scopus rating (2011): SJR 2.501 SNIP 1.454 CiteScore 5.69

ISI indexed (2011): ISI indexed no

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Relating Magnetic Properties and High Hyperthermia Performance of Iron Oxide Nanoflowers

We investigated in depth the interrelations among structure, magnetic properties, relaxation dynamics and magnetic hyperthermia performance of magnetic nanoflowers. The nanoflowers are about 39 nm in size, and consist of densely packed iron oxide cores. They display a remanent magnetization, which we explain by the exchange coupling between the cores, but we observe indications for internal spin disorder. By polarized small angle neutron scattering we unambiguously confirm that on average the nanoflowers are preferentially magnetized along one direction. The extracted discrete relaxation time distribution of the colloidally dispersed particles indicates the presence of three distinct relaxation contributions. We can explain the two slower processes by Brownian and classical Néel relaxation, respectively. The additionally observed very fast relaxation contributions are attributed by us to the relaxation of the disordered spins within the nanoflowers. Finally, we show that the intrinsic loss power (ILP, magnetic hyperthermia performance) of the nanoflowers measured in colloidal dispersion at high frequency is comparatively large and independent of the viscosity of the surrounding medium. This concurs with our assumption that the observed relaxation in the high frequency range is primarily a result of internal spin relaxation, and probably connected to the disordered spins within the individual nanoflowers.

General information
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Organisations: Department of Micro- and Nanotechnology, Magnetic Systems, Department of Physics, Neutrons and X-rays for Materials Physics, Universidad de Cantabria, Technische Universität Braunschweig, Physikalisch-Technische Bundesanstalt, Uppsala University, University College London, Federal Institute for Materials Research and Testing, Chalmers University of Technology, University of Rostock, Micromod Partikeltechnologie GmbH, Institut Laue-Langevin, RISE Acreo
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Main Research Area: Technical/natural sciences

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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SJR 2.135 SNIP 1.147 CiteScore 4.58
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
Rich Ground State Chemical Ordering in Nanoparticles: Exact Solution of a Model for Ag-Au Clusters

We show that nanoparticles can have very rich ground state chemical order. This is illustrated by determining the chemical ordering of Ag-Au 309-atom Mackay icosahedral nanoparticles. The energy of the nanoparticles is described using a cluster expansion model, and a Mixed Integer Programming (MIP) approach is used to find the exact ground state configurations for all stoichiometries. The chemical ordering varies widely between the different stoichiometries, and display a rich zoo of structures with non-trivial ordering.

General information
State: Accepted/In press
Organisations: Department of Physics, Theoretical Atomic-scale Physics
Authors: Larsen, P. M. (Intern), Jacobsen, K. W. (Intern), Schiøtz, J. (Intern)
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Main Research Area: Technical/natural sciences

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BFI (2018): BFI-level 2
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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
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 at high polarization will be summarised.
Scalable Synthesis of Carbon-Supported Platinum–Lanthane and Rare-Earth Alloys for Oxygen Reduction

Platinum–rare-earth alloys have proven to be both active and stable under accelerated stability tests in their bulk polycrystalline form. However, a scalable method for the synthesis of a high-surface-area supported catalyst of these alloys has so far not been presented. Herein we discuss the thermodynamics relevant for the reduction conditions of the rare earths to form alloys with platinum. We show how the tolerance for water and oxygen severely limits the synthesis parameters and how under certain conditions the thermal reduction of YCl₃ with H₂ is possible from 500 °C. From the insight gained, we synthesized a PtₓY/C catalyst by modifying a Pt/C catalyst and confirmed alloy formation by both X-ray diffraction and X-ray photoelectron spectroscopy measurements. These reveal crystalline intermetallic phases and the metallic state of yttrium. Without any optimization of the method, the catalyst has an improved mass activity in comparison to the unmodified catalyst, proving the viability of the method. Initial work based on thermodynamic equilibrium calculations on reduction time show promise in controlling the phase formed by tuning the parameters of time, temperature, and gas composition.

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Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics, Center for Electron Nanoscopy, Danish Technological Institute
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Volume: 8
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BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 2.113 SJR 4.921 CiteScore 11.49
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
Scattering of flexural waves in Euler-Bernoulli beams by short-range potentials: Paper

Time-harmonic flexural waves on a beam and on two elastically coupled beams with short-range localized imperfections in the mass distribution and in the position dependent coupling are considered. Thus scattering of an incident wave solution to the Euler-Bernoulli equation by a Dirac delta function and its derivative up to order three is studied, and the possible physical interpretations are outlined. Reflected, transmitted and evanescent waves exist, and their scattering data are determined. For δ(x) and δ'(x), the scattering problem is solved by standard integration. For δ''(x) and δ'''(x), the standard integration procedure does not work and solutions are obtained by regularization. In the latter case the scatterer is in general nontransparent and only partially penetrable at discrete resonances. The first few of these as well as their scattering data are determined numerically.

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Department of Physics, Dynamical Systems, Bogolyubov Institute for Theoretical Physics Nasu
Authors: Christiansen, P. L. (Intern), Iermakova, S. V. (Ekstern), Gaididei, Y. B. (Ekstern), Sørensen, M. P. (Intern)
Number of pages: 16
Publication date: 2018
Main Research Area: Technical/natural sciences

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Journal: Journal of Physics A-mathematical and Theoretical
Volume: 51
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Article number: 095202
ISSN (Print): 1751-8113
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 0.924 SJR 0.843 CiteScore 1.74
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.45 SJR 0.935 SNIP 0.959
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.028 SNIP 1.048 CiteScore 1.34
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.936 SNIP 0.945 CiteScore 1.36
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.935 SNIP 0.998 CiteScore 1.42
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Selective CO Methanation on Highly Active Ru/TiO₂ Catalysts: Identifying the Physical Origin of the Observed Activation/Deactivation and Loss in Selectivity

Ru/TiO₂ catalysts are highly active and selective in the selective methanation of CO in the presence of large amounts of CO₂, but suffer from a considerable deactivation and loss of selectivity during time on stream. Aiming at a fundamental understanding of these processes, we have systematically investigated the physical reasons responsible for these effects, using catalysts with different surface areas and combining time resolved kinetic and in situ / operando spectroscopy measurements as well as ex situ catalyst characterization. This allowed us to identify and disentangle contributions from different effects such as structural effects, adlayer effects such as site blocking effects and changes in the chemical (surface) composition of the catalysts. Operando XANES / EXAFS measurements revealed that an initial activation phase is largely due to the reduction of oxidized Ru species, together with a distinct change in the Ru particle shape, until reaching a state dominated by metallic Ru species (fraction RuO₂

General information

State: Published
Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics, University of Ulm
Authors: Abdel-Mageed, A. M. (Ekstem), Widmann, D. (Ekstem), Olesen, S. E. (Intern), Chorkendorff, I. (Intern), Behm, R. J. (Ekstem)
Number of pages: 16
Pages: S399-5414
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information

Journal: A C S Catalysis
Volume: 8
Simulation tools for detector and instrument design
The high performance requirements at the European Spallation Source have been driving the technological advances on the neutron detector front. Now more than ever is it important to optimize the design of detectors and instruments, to fully exploit the ESS source brilliance. Most of the simulation tools the neutron scattering community has at their disposal target the instrument optimization until the sample position, with little focus on detectors. The ESS Detector Group has extended the capabilities of existing detector simulation tools to bridge this gap. An extensive software framework has been developed, enabling efficient and collaborative developments of required simulations and analyses – based on the use of the Geant4 Monte Carlo toolkit, but with extended physics capabilities where relevant (like for Bragg diffraction of thermal neutrons in crystals). Furthermore, the MCPL (Monte Carlo Particle Lists) particle data exchange file format, currently supported for the primary Monte Carlo tools of the community (McStas, Geant4 and MCNP), facilitates the integration of detector simulations with existing simulations of instruments using these software packages. These means offer a powerful set of tools to tailor the detector and instrument design to the instrument application.

General information
State: Accepted/In press
Organisations: Center for Nuclear Technologies, Radiation Physics, Department of Physics, Neutrons and X-rays for Materials Physics, European Spallation Source ESS AB, Mid Sweden University
Authors: Kanaki, K. (Ekstern), Kittelmann, T. (Ekstern), Cai, X. X. (Intern), Klinkby, E. B. (Intern), Knudsen, E. B. (Intern), Willendrup, P. K. (Intern), Hall-Wilton, R. (Ekstern)
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information
Journal: Physica B: Condensed Matter
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Ratings:
BFI (2018): BFI-level 1
Simulation tools for scattering corrections in spectrally resolved X-ray Computed Tomography using McXtrace

Spectral computed tomography is an emerging imaging method that involves using recently developed energy discriminating photon-counting detectors (PCDs). This technique enables measurements at isolated high-energy ranges, in which the dominating undergoing interaction between the x-ray and the sample is the incoherent scattering. The
scattered radiation causes a loss of contrast in the results, and its correction has proven to be a complex problem, due to its dependence on energy, material composition, and geometry. Monte Carlo simulations can utilize a physical model to estimate the scattering contribution to the signal, at the cost of high computational time. We present a fast Monte Carlo simulation tool, based on McXtrace, to predict the energy resolved radiation being scattered and absorbed by objects of complex shapes. We validate the tool through measurements using a CdTe single PCD (Multix ME-100) and use it for scattering correction in a simulation of a spectral CT. We found the correction to account for up to 7% relative amplification in the reconstructed linear attenuation. It is a useful tool for x-ray CT to obtain a more accurate material discrimination, especially in the high-energy range, where the incoherent scattering interactions become prevailing (>50keV).

**General information**
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Department of Applied Mathematics and Computer Science, Image Analysis & Computer Graphics, University of Copenhagen
Authors: Busi, M. (Intern), Olsen, U. L. (Intern), Knudsen, E. B. (Intern), Frisvad, J. R. (Intern), Kehres, J. (Intern), Dreier, E. S. (Ekstern)
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Publication date: 2018
Main Research Area: Technical/natural sciences

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BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 0.746 SJR 0.424 CiteScore 1.12
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.11 SJR 0.42 SNIP 0.823
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.474 SNIP 0.924 CiteScore 1.03
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.458 SNIP 1.04 CiteScore 1
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.485 SNIP 1.031 CiteScore 1.03
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.484 SNIP 0.909 CiteScore 0.84
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.471 SNIP 0.966 CiteScore 0.91
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.442 SNIP 0.931
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.47 SNIP 0.88
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.472 SNIP 0.888
Scopus rating (2007): SJR 0.559 SNIP 0.897
Solvent control of charge transfer excited state relaxation pathways in [Fe(2,2'-bipyridine)(CN)₄]²⁻

The excited state dynamics of solvated [Fe(bpy)(CN)₄]²⁻, where bpy = 2,2'-bipyridine, show significant sensitivity to the solvent Lewis acidity. Using a combination of optical absorption and X-ray emission transient spectroscopies, we have previously shown that the metal to ligand charge transfer (MLCT) excited state of [Fe(bpy)(CN)₄]²⁻ has a 19 picosecond lifetime and no discernable contribution from metal centered (MC) states in weak Lewis acid solvents, such as dimethyl sulfoxide and acetonitrile. In the present work, we use the same combination of spectroscopic techniques to measure the MLCT excited state relaxation dynamics of [Fe(bpy)(CN)₄]²⁻ in water, a strong Lewis acid solvent. The charge-transfer excited state is now found to decay in less than 100 femtoseconds, forming a quasi-stable metal centered excited state with a 13 picosecond lifetime. We find that this MC excited state has triplet (3MC) character, unlike other reported six-coordinate Fe(II)-centered coordination compounds, which form MC quintet (5MC) states. The solvent dependent changes in excited state non-radiative relaxation for [Fe(bpy)(CN)₄]²⁻ allows us to infer the influence of the solvent on the electronic structure of the complex. Furthermore, the robust characterization of the dynamics and optical spectral signatures of the isolated 3MC intermediate provides a strong foundation for identifying 3MC intermediates in the electronic excited state relaxation mechanisms of similar Fe-centered systems being developed for solar applications.

General information

State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, SLAC National Accelerator Laboratory, Stanford University, Lund University, Hungarian Academy of Sciences, Deutsches Elektronen-Synchrotron
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Main Research Area: Technical/natural sciences

Publication information
Journal: Physical Chemistry Chemical Physics
Volume: 20
Issue number: 6
ISSN (Print): 1463-9076
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BFI (2018): BFI-level 2
Spin-Orbital Excitations in Ca$_2$RuO$_4$ Revealed by Resonant Inelastic X-Ray Scattering
The strongly correlated insulator Ca$_2$RuO$_4$ is considered as a paradigmatic realization of both spin-orbital physics and a band-Mott insulating phase, characterized by orbitally selective coexistence of a band and a Mott gap. We present a high resolution oxygen K-edge resonant inelastic x-ray scattering study of the antiferromagnetic Mott insulating state of Ca$_2$RuO$_4$. A set of low-energy (about 80 and 400 meV) and high-energy (about 1.3 and 2.2 eV) excitations are reported, which show strong incident light polarization dependence. Our results strongly support a spin-orbit coupled band-Mott scenario and explore in detail the nature of its exotic excitations. Guided by theoretical modeling, we interpret the low-energy excitations as a result of composite spin-orbital excitations. Their nature unveils the intricate interplay of crystal-field splitting and spin-orbit coupling in the band-Mott scenario. The high-energy excitations correspond to intra-atomic singlet-triplet transitions at an energy scale set by Hund's coupling. Our findings give a unifying picture of the spin and orbital excitations in the band-Mott insulator Ca$_2$RuO$_4$. 

General information
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Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Universität Zürich, Universita di Salerno, Ecole Polytechnique Federale de Lausanne (EPFL), Technical University of Denmark, Paul Scherrer Institut, National Institute for Materials Science
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BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 3.073 SJR 6.11 CiteScore 11.47
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 10.08 SJR 7.434 SNIP 3.214
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 6.568 SNIP 2.334 CiteScore 6.23
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 8.101 SNIP 2.924 CiteScore 7.74
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 7.335 SNIP 2.804 CiteScore 7.7
ISI indexed (2013): ISI indexed yes
Scopus rating (2012): SJR 7.632 SNIP 1.806 CiteScore 6.08
ISI indexed (2012): ISI indexed no
ISI indexed (2011): ISI indexed no
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Stability of charge-stripe ordered La$_{2-x}$Sr$_x$NiO$_{4+\delta}$ at one third doping

The stability of charge ordered phases is doping dependent, with different materials having particularly stable ordered phases. In the half filled charge ordered phases of the cuprates this occurs at one eighth doping, whereas in charge-stripe ordered La$_{2-x}$Sr$_x$NiO$_{4+\delta}$ there is enhanced stability at one third doping. In this paper we discuss the known details of the charge-stripe order in La$_{2-x}$Sr$_x$NiO$_{4+\delta}$, and how these properties lead to the one third doping stability.
The stability of charge ordered phases is doping dependent, with different materials having particularly stable ordered phases. In the half filled charge ordered phases of the cuprates this occurs at one eighth doping, whereas in charge-stripe ordered La$_{2-x}$Sr$_x$NiO$_{4+\delta}$ there is enhanced stability at one third doping. In this paper we discuss the known details of the charge-stripe order in La$_{2-x}$Sr$_x$NiO$_{4+\delta}$, and how these properties lead to the one third doping stability.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, University of Central Lancashire, Technische Universität München, Institut Laue-Langevin, University of Oxford
Authors: Freeman, P. G. (Ekstern), Mole, R. A. (Ekstern), Christensen, N. B. (Intern), Stunault, A. (Ekstern), Prabhakaran, D. (Ekstern)
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Main Research Area: Technical/natural sciences

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Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 0.791 SJR 0.417 CiteScore 1.45
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
Stable source reconstruction from a finite number of measurements in the multi-frequency inverse source problem

We consider the multi-frequency inverse source problem for the scalar Helmholtz equation in the plane. The goal is to reconstruct the source term in the equation from measurements of the solution on a surface outside the support of the source. We study the problem in a certain finite dimensional setting: From measurements made at a finite set of frequencies we uniquely determine and reconstruct sources in a subspace spanned by finitely many Fourier-Bessel functions. Further, we obtain a constructive criterion for identifying a minimal set of measurement frequencies sufficient for reconstruction, and under an additional, mild assumption, the reconstruction method is shown to be stable. Our analysis is based on a singular value decomposition of the source-to-measurement forward operators and the distribution of positive zeros of the Bessel functions of the first kind. The reconstruction method is implemented numerically and our theoretical findings are supported by numerical experiments.

General information

State: Published
Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, Neutrons and X-rays for Materials Physics
Authors: Karamehmedovic, M. (Intern), Kirkeby, A. (Intern), Knudsen, K. (Intern)
Number of pages: 24
Publication date: 2018
Main Research Area: Technical/natural sciences
Structural Evaluation of 5,5′-Bis(naphth-2-yl)-2,2′-bithiophene in Organic Field-Effect Transistors with n-Octadecytrichlorosilane Coated SiO$_2$ Gate Dielectric
We report on the structure and morphology of 5,5′-bis(naphth-2-yl)-2,2′-bithiophene (NaT2) films in bottom-contact organic field-effect transistors (OFETs) with octadecyltrichlorosilane (OTS) coated SiO2 gate dielectric, characterized by atomic force microscopy (AFM), grazing-incidence X-ray diffraction (GIXRD), and electrical transport measurements. Three types of devices were investigated with the NaT2 thin-film deposited either on (1) pristine SiO2 (corresponding to higher surface energy, 47 mJ/m²) or on OTS deposited on SiO2 under (2) anhydrous or (3) humid conditions (corresponding to lower surface energies, 20–25 mJ/m²). NaT2 films grown on pristine SiO2 form nearly featureless three-dimensional islands. NaT2 films grown on OTS/SiO2 deposited under anhydrous conditions form staggered pyramid islands where the interlayer spacing corresponds to the size of the NaT2 unit cell. At the same time, the grain size measured by AFM increases from hundreds of nanometers to micrometers and the crystal size measured by GIXRD from 30 nm to more than 100 nm. NaT2 on OTS/SiO2 deposited under humid conditions also promotes staggered pyramids but with smaller crystals 30–80 nm. The NaT2 unit cell parameters in OFETs differ 1–2% from those in bulk. Carrier mobilities tend to be higher for NaT2 layers on SiO2 (2–3 × 10–4 cm²/(V s)) compared to NaT2 on OTS (2 × 10–5–1 × 10–4 cm²/(V s)). An applied voltage does not influence the unit cell parameters when probed by GIXRD in operando.

General information
State: Accepted/In press
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Technical University of Denmark, European Synchrotron Radiation Facility, Syddansk Universitet
Authors: Lauritzen, A. E. (Ekstern), Torkkeli, M. (Intern), Bikondoa, O. (Ekstern), Linnet, J. (Forskerdatabase), Tavares, L. (Forskerdatabase), Kjelstrup-Hansen, J. (Forskerdatabase), Knaapila, M. (Intern)
Publication date: 2018
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Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): SJR 1.479 SNIP 1.148 CiteScore 4
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.99 SJR 1.559 SNIP 1.178
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.65 SNIP 1.281 CiteScore 4.33
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.81 SNIP 1.371 CiteScore 4.59
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.896 SNIP 1.343 CiteScore 4.55
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 2.179 SNIP 1.369 CiteScore 4.37
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 2.051 SNIP 1.349 CiteScore 4.42
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 2.158 SNIP 1.393
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.164 SNIP 1.344
57Fe-Mössbauer spectroscopy and electrochemical activities of graphitic layer encapsulated iron electrocatalysts for the oxygen reduction reaction

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 ⁵⁷Fe-Mössbauer spectroscopy the iron containing components were identified including α-Fe, γ-Fe, γ-Fe₂O₃, and Fe₃C as well as a minor doublet component due to Fe³⁺ in high spin and/or Fe²⁺ 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 Fe₃C content in the range of study, indicating involvement of the encapsulated nanoparticles in the ORR catalysis. The reognition 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.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Department of Physics, Neutrons and X-rays for Materials Physics, Proton conductors
Authors: Zhong, L. (Intern), Frandsen, C. (Intern), Mørup, S. (Intern), Hu, Y. (Intern), Pan, C. (Intern), Cleemann, L. N. (Intern), Jensen, J. O. (Intern), Li, Q. (Intern)
Number of pages: 7
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Main Research Area: Technical/natural sciences

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Journal: Applied Catalysis B: Environmental
Volume: 221
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Ratings:
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57Fe-Mössbauer spectroscopy, Encapsulated Fe catalysts, Fuel cells, Oxygen reduction reaction

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Source-ID: 2391035353
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The fractional Fourier transform as a simulation tool for lens-based X-ray microscopy

The fractional Fourier transform (FrFT) is introduced as a tool for numerical simulations of X-ray wavefront propagation. By removing the strict sampling requirements encountered in typical Fourier optics, simulations using the FrFT can be carried out with much decreased detail, allowing, for example, on-line simulation during experiments. Moreover, the additive index property of the FrFT allows the propagation through multiple optical components to be simulated in a single step, which is particularly useful for compound refractive lenses (CRLs). It is shown that it is possible to model the attenuation from the entire CRL using one or two effective apertures without loss of accuracy, greatly accelerating simulations involving CRLs. To demonstrate the applicability and accuracy of the FrFT, the imaging resolution of a CRL-based imaging system is estimated, and the FrFT approach is shown to be significantly more precise than comparable approaches using geometrical optics. Secondly, it is shown that extensive FrFT simulations of complex systems involving coherence and/or nonmonochromatic sources can be carried out in minutes. Specifically, the chromatic aberrations as a function of source bandwidth are estimated, and it is found that the geometric optics greatly overestimates the aberration for energy bandwidths of around 1%.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, European Synchrotron Radiation Facility
Authors: Pedersen, A. F. (Intern), Simons, H. (Intern), Detlefs, C. (Ekstern), Poulsen, H. F. (Intern)
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Journal: Journal of Synchrotron Radiation
Volume: 25
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Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 1.431 SJR 1.65 CiteScore 3.12
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.86 SJR 1.521 SNIP 1.491
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.146 SNIP 1.301 CiteScore 2.45
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.317 SNIP 1.477 CiteScore 2.58
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.476 SNIP 1.676 CiteScore 2.91
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.465 SNIP 1.261 CiteScore 2.36
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.736 SNIP 1.403 CiteScore 2.45
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.629 SNIP 1.466
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.507 SNIP 1.386
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
The Generalized Multipole Technique for the Simulation of Low-Loss Electron Energy Loss Spectroscopy

In this study, we demonstrate the use of a Generalized Multipole Technique (GMT) to simulate low-loss Electron Energy Loss Spectroscopy (EELS) spectra of isolated spheroidal nanoparticles. The GMT provides certain properties, such as semi-analytical description of the electromagnetic fields, efficient solution of the underlying electromagnetic model, accurate description of the near field, and flexibility regarding the position and direction of the incident electron beam, that are advantageous for computation of EELS spectra. Within the chapter, we provide a derivation of the electromagnetic model and its connection to EELS spectra, and comprehensive validation of the implemented GMT regarding electromagnetic scattering and EELS.

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, Neutrons and X-rays for Materials Physics, University of Bremen
Authors: Kiewidt, L. (Ekstern), Karamehmedovic, M. (Intern)
Pages: 147-167
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Publisher: Springer
Editors: Wriedt, T., Eremin, Y.
ISBN (Print): 978-3-319-74889-4
Chapter: 7

The Importance of Surface IrOx in Stabilizing RuO2 for Oxygen Evolution
The high precious metal loading and high overpotential of the oxygen evolution reaction (OER) prevents the widespread utilization of polymer electrolyte membrane (PEM) water electrolyzers. Herein we explore the OER activity and stability in acidic electrolyte of a combined IrOx/RuO2 system consisting of RuO2 thin films with sub-monolayer (1, 2 and 4 Å)
amounts of IrO$_x$ deposited on top. Operando extended X-ray absorption fine structure (EXAFS) on the Ir L-3 edge revealed a rutile type IrO$_2$ structure with some Ir sites occupied by Ru, IrO$_x$ being at the surface of the RuO$_2$ thin film. We monitor corrosion on IrO$_x$/RuO$_2$ thin films by combining electrochemical quartz crystal microbalance (EQCM) with inductively coupled mass spectrometry (ICP-MS). We elucidate the importance of sub-monolayer surface IrO$_x$ in minimizing Ru dissolution. Our work shows that we can tune the surface properties of active OER catalysts such as RuO$_2$, aiming to achieve higher electrocatalytic stability in PEM electrolyzers.
The Melting Curve of Nickel Up to 100 GPa Explored by XAS

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, European Synchrotron Radiation Facility, Ehime University, Diamond Light Source Ltd, Sorbonne Universités
Authors: Boccato, S. (Ekstern), Torchio, R. (Ekstern), Kantor, I. (Intern), Morard, G. (Ekstern), Anzellini, S. (Ekstern), Giampaoli, R. (Ekstern), Briggs, R. (Ekstern), Smareglia, A. (Ekstern), Irifune, T. (Ekstern), Pascarelli, S. (Ekstern)
Pages: 9921–9930
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Main Research Area: Technical/natural sciences

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Journal: Journal of Geophysical Research: Solid Earth
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): SJR 2.272 SNIP 1.475 CiteScore 3.19
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.36 SJR 2.369 SNIP 1.558
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 2.754 SNIP 1.605 CiteScore 3.39
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.853 SNIP 1.757 CiteScore 3.27
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 3.088 SNIP 1.809 CiteScore 3.38
Acoustofluidics is the combined science of acoustics and microfluidics. In acoustofluidics, ultrasound acoustic waves are used to generate forces for manipulation of fluids and particles in networks of microchannels in a microfluidic chip. The microscale systems are designed to enable fundamentally new capabilities in chemical, biomedical, or clinical studies of single cells and bioparticles.

This thesis, entitled Theory of nonlinear acoustic forces acting on fluids and particles in microsystems, advances the fundamental understanding of acoustofluidics by addressing the origin of the nonlinear acoustic forces acting on fluids and particles. Classical results in nonlinear acoustics for the non-dissipative acoustic radiation force acting on a particle or an interface, as well as the dissipative acoustic force densities driving acoustic streaming, are derived and discussed in terms of a single principal equation. This principal equation relates the acoustic force density to the divergence in the acoustic (pseudo-)momentum-flux-density tensor, dependent only on the linear acoustic fields. Extending the principal equation to the case of an inhomogeneous fluid with variations in the continuous fluid parameters.
of density and compressibility, e.g., due to a solute concentration field, the thesis presents novel analytical results on the acoustic force density acting on inhomogeneous fluids in acoustic fields. This inhomogeneity-induced acoustic force density is non-dissipative in origin, in contrast to the force densities driving acoustic streaming in a homogeneous fluid. It depends on the linear acoustic fields and the gradients in the fluid density and compressibility, and leads to a dynamic relocation and stabilization of inhomogeneities in acoustic fields, as demonstrated by simulations as well as experiments with aqueous solutions in an acoustofluidic glass-silicon microchip.

The ability of the acoustic force density to stabilize fluid inhomogeneities makes possible the development of a microfluidic analog to density-gradient centrifugation, called iso-acoustic focusing, which is demonstrated for acousto-mechanical phenotyping of single white blood cells and cancer cells in continuous flow. The theory of the acoustic force density furthermore leads to the prediction of the possibility of using acoustic tweezers to actively manipulate miscible-fluid interfaces and concentration fields at the microscale. Experimental work in progress verifies the validity of this prediction. Finally, boundary-driven acoustic streaming, historically limited to the study of homogeneous fluids, is brought into the realm of inhomogeneous fluids in a theoretical, numerical, and experimental study of acoustic streaming in inhomogeneous fluids. The study presents the discovery and description of a new class of suppressed acoustic streaming flows resulting from the competition between the classical dissipative boundary-driven acoustic force density and the inhomogeneity-induced acoustic force density that stabilizes the inhomogeneity configuration, thereby suppressing the advective streaming flow. The suppressed acoustic streaming flow evolves towards the well-known boundary-driven streaming pattern, as the acoustically stabilized inhomogeneity profile flattens by diffusion and advection on a one-minute time scale.

More theoretical and experimental work is needed to fully understand the implications of the theory of acoustofluidics in inhomogeneous fluids presented in this thesis, and I can only hope that this thesis will inspire such research activities.
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.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Department of Energy Conversion and Storage, Imaging and Structural Analysis, Department of Applied Mathematics and Computer Science, Image Analysis & Computer Graphics, University of Copenhagen, Japan Atomic Energy Agency, University of California at Berkeley, University of Manchester
Authors: Sales, M. (Intern), Strobl, M. (Ekstern), Shinohara, T. (Ekstern), Tremsin, A. (Ekstern), Kuhn, L. T. (Intern), Lionheart, W. R. B. (Ekstern), Desai, N. M. (Ekstern), Dahl, A. B. (Intern), Schmidt, S. (Intern)
Pages: 1-6
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information
Journal: Scientific Reports
Volume: 8
Issue number: 1
Article number: 2214
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
Tomography of a displacement photon counter for discrimination of single-rail optical qubits

We investigate the performance of a detection strategy composed of a displacement operation and a photon counter, which is known as a beneficial tool in optical coherent communications, to the quantum state discrimination of the two superpositions of vacuum and single photon states corresponding to the eigenstates in the single-rail encoding of photonic qubits. We experimentally characterize the detection strategy in vacuum-single photon two-dimensional space using quantum detector tomography and evaluate the achievable discrimination error probability from the reconstructed measurement operators. We furthermore derive the minimum error rate obtainable with Gaussian transformations and homodyne detection. Our proof-of-principle experiment shows that the proposed scheme can achieve a discrimination error surpassing homodyne detection.

General information
State: Published
Organisations: Department of Physics, Quantum Physics and Information Technology
Authors: Izumi, S. (Intern), Neergaard-Nielsen, J. S. (Intern), Andersen, U. L. (Intern)
Number of pages: 5
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Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Physics B: Atomic, Molecular and Optical Physics
Volume: 51
Issue number: 8
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): SNIP 0.884 SJR 0.85 CiteScore 1.77
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 1.22 SJR 0.781 SNIP 0.759
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.025 SNIP 1.023 CiteScore 1.19
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.192 SNIP 0.951 CiteScore 1.5
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.119 SNIP 0.971 CiteScore 1.62
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.245 SNIP 1.112 CiteScore 1.63
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.061 SNIP 0.932 CiteScore 1.7
ISI indexed (2011): ISI indexed yes
Research in fusion energy seeks to develop a green, safe, and sustainable energy source. Nuclear fusion can be achieved by heating a hydrogen gas to temperatures of millions of kelvin. At fusion temperatures, some or all the electrons leave the atomic nucleus of the hydrogen atom. This results in an overall neutral gaseous state of negatively charged free electrons and positively charged ions. This state of matter is called plasma. To achieve and maintain fusion temperatures, the plasma must avoid direct contact with any solid material. Since the plasma consists of charged particles, it can be confined with an appropriate configuration of strong magnetic fields. Toroidal magnetic confinement devices, such as the tokamak, are the most promising designs for a fusion reactor. A tokamak can operate in two distinct modes of operation. These are the low confinement mode (L-mode) and the high confinement mode (H-mode). H-mode is the preferred operating mode for a fusion reactor. The transition from L-mode to H-mode is called the L–H transition. The confinement properties of a plasma are largely determined by the physics near the edge of the confinement region of the plasma. The edge transport of a magnetically confined plasma is predominantly caused by recurring bursts of coherent plasma structures. These structures are in L-mode called blob filaments (blobs) and in H-mode categorized into edge localized mode (ELM) filaments or inter-ELM filaments. To improve the plasma confinement, it is important to understand the evolution of these structures. We apply a dynamical systems approach to quantitatively describe the time evolution of these state variables. A critical point of a variable defines a feature point where that variable is significant. For a range of Rayleigh and Prandtl numbers, we analyze the bifurcations of the critical points of the three variables with time as the main bifurcation parameter. Plasma simulations can be computationally demanding. We apply a Galerkin method to approximate a plasma convection model with a reduced model. The time evolution of the energies of the pressure profile, the turbulent flow, and the zonal flow capture the dynamic behavior of the convection model. Rayleigh decomposition splits the variables of the model into averaged variables and fluctuation variables. We approximate the fluctuation variables by truncated Fourier series and project the equations onto the Fourier basis functions. This results in a computationally simpler model with the spatial dimension reduced by one. Bifurcation diagrams for the energies show consistency between the bifurcation structures of the full and the reduced model.

Finally, we utilize a data-driven modeling approach called SINDy to identify a reduced model from simulation data of a convection model. The reduced model reveals a predator-prey relationship between the zonal flow energy and the turbulent energy. The analytically derived bifurcation diagram for the reduced model has the same structure as the data-based bifurcation diagram for the full model.
Layered transition metal dichalcogenides have distinct physicochemical properties at their edge-terminations. The production of an abundant density of edge structures is, however, impeded by the excess surface energy of edges compared to basal planes and would benefit from insight into the atomic growth mechanisms. Here, we show that edge-terminated MoS$_2$ nanostructures can form during sulfidation of MoO$_2$ nanocrystals by using in situ transmission electron microscopy (TEM). Time-resolved TEM image series reveal that the MoO$_2$ surface can sulfide by inward progression of MoO$_2$(20-2):MoS$_2$(002) interfaces resulting in upright-oriented and edge-exposing MoS$_2$ sheets. This topotactic growth is rationalized in interplay with density functional theory calculations by successive O-S exchange and Mo sublattice restructuring steps. The analysis shows that e-MoS$_2$ formation is energetically favorable at MoO$_2$(110) surfaces and provides a necessary requirement for the propensity of a specific MoO$_2$ surface termination to form edge-terminated MoS$_2$. Thus, the present findings should benefit the rational development of transition metal dichalcogenide nanomaterials with abundant edge-terminations.
Toward the Decentralized Electrochemical Production of H$_2$O$_2$: A Focus on the Catalysis

H$_2$O$_2$ is a valuable, environmentally friendly oxidizing agent, with a wide range of uses, from the provision of clean water to the synthesis of valuable chemicals. The on-site electrolytic production of H$_2$O$_2$ would bring the chemical to applications beyond its present reach. The successful commercialization of electrochemical H$_2$O$_2$ production requires cathode catalysts with high activity, selectivity and stability. In this Perspective, we highlight our current understanding of the factors that control the cathode performance. We review the influence of catalyst material, electrolyte and the structure of the interface at the mesoscopic scale. We provide original theoretical data on the role of the geometry of the active site and its influence on activity and selectivity. We have also conducted a series of original experiments on (i) the effect of pH on H$_2$O$_2$ production on glassy carbon, pure metals, and metal-mercury alloys, and (ii) the influence of cell geometry and mass transport in liquid half-cells in comparison to membrane electrode assemblies.
Tracking the picosecond deactivation dynamics of a photoexcited iron carbene complex by time-resolved X-ray scattering

Recent years have seen the development of new iron-centered N-heterocyclic carbene (NHC) complexes for solar energy applications. Compared to typical ligand systems, the NHC ligands provide Fe complexes with longer-lived metal-to-ligand charge transfer (MLCT) states. This increased lifetime is ascribed to strong ligand field splitting provided by the NHC ligands that raises the energy levels of the metal centered (MC) states and therefore reduces the deactivation efficiency of MLCT states. Among currently known NHC systems, \([\text{Fe(btbip)}_2]^{2+}\) (btbip = 2,6-bis(3-tert-butyl-imidazol-1-ylidine)pyridine) is a unique complex as it exhibits a short-lived MC state with a lifetime on the scale of a few hundreds of picoseconds. Hence, this complex allows for a detailed investigation, using 100 ps X-ray pulses from a synchrotron, of strong ligand field effects on the intermediate MC state in an NHC complex. Here, we use time-resolved wide angle X-ray scattering (TRWAXS) aided by density functional theory (DFT) to investigate the molecular structure, energetics and lifetime of the high-energy MC state in the Fe-NHC complex \([\text{Fe(btbip)}_2]^{2+}\) after excitation to the MLCT manifold. We identify it as a 260 ps metal-centered quintet (\(^5\)MC) state, and we refine the molecular structure of the excited-state complex verifying the DFT results. Using information about the hydrodynamic state of the solvent, we also determine, for the first time, the energy of the \(^5\)MC state as 0.75 \pm 0.15 eV. Our results demonstrate that due to the increased ligand field strength caused by NHC ligands, upon transition from the ground state to the \(^5\)MC state, the metal to ligand bonds extend by unusually large values: by 0.29 ångstrom in the axial and 0.21 ångstrom in the equatorial direction. These results imply that the transition in the photochemical properties from typical Fe complexes to novel NHC compounds is manifested not only in the destabilization of the MC states, but also in structural distortion of these states.

**General information**

State: Published
Organisations: Neutrons and X-rays for Materials Physics, Department of Physics, European Synchrotron Radiation Facility, Lund University, European XFEL
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**Publication information**

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- Web of Science (2018): Indexed yes
- BFI (2017): BFI-level 1
- Scopus rating (2017): SNIP 1.666 SJR 4.508 CiteScore 8.54
- Web of Science (2017): Indexed yes
- BFI (2016): BFI-level 1
Unbiased, complete solar charging of a neutral flow battery by a single Si photocathode

Solar redox flow batteries have attracted attention as a possible integrated technology for simultaneous conversion and storage of solar energy. In this work, we review current efforts to design aqueous solar flow batteries in terms of battery electrolyte capacity, solar conversion efficiency and depth of solar charge. From a materials cost and design perspective, a simple, cost-efficient, aqueous solar redox flow battery will most likely incorporate only one semiconductor, and we demonstrate here a system where a single photocathode is accurately matched to the redox couples to allow for a complete solar charge. The single TiO$_2$ protected Si photocathode with a catalytic Pt layer can fully solar charge a neutral TEMPO-sulfate/ferricyanide battery with a cell voltage of 0.35 V. An unbiased solar conversion efficiency of 1.6% is obtained and this system represents a new strategy in solar RFBs where a single silicon photocathode is paired with energetically suitable redox couples to build an integrated solar energy conversion and storage device with full realization of the energy storage capacity.
Viscous flow in a soft valve

Fluid-structure interactions are ubiquitous in nature and technology. However, the systems are often so complex that numerical simulations or ad hoc assumptions must be used to gain insight into the details of the complex interactions between the fluid and solid mechanics. In this paper, we present experiments and theory on viscous flow in a simple bioinspired soft valve which illustrate essential features of interactions between hydrodynamic and elastic forces at low Reynolds numbers. The set-up comprises a sphere connected to a spring located inside a tapering cylindrical channel. The spring is aligned with the central axis of the channel and a pressure drop is applied across the sphere, thus forcing the liquid through the narrow gap between the sphere and the channel walls. The sphere’s equilibrium position is determined by a balance between spring and hydrodynamic forces. Since the gap thickness changes with the sphere’s position, the system has a pressure-dependent hydraulic resistance. This leads to a nonlinear relation between applied pressure and flow rate: flow initially increases with pressure, but decreases when the pressure exceeds a certain critical value as the gap closes. To rationalize these observations, we propose a mathematical model that reduced the complexity of the flow to a two-dimensional lubrication approximation. A closed-form expression for the pressure drop/flow rate is obtained which reveals that the flow rate $Q$ depends on the pressure drop $\Delta p$, sphere radius $a$, gap thickness $h_0$, and viscosity $\eta$ as $Q \sim \eta^{-1} a^{1/2} h_0^{5/2} (1 - \Delta p/\Delta p_c)^{5/2} \Delta p$, where the critical pressure $\Delta p_c$ scales with spring constant $k$ as $\Delta p_c \sim kh_0 a^{-2}$. These predictions compared favourably to the results of our experiments with no free parameters.
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Scopus rating (2017): SJR 1.591 SNIP 1.702 CiteScore 3.33
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.82 SJR 1.744 SNIP 1.671
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.896 SNIP 1.639 CiteScore 2.57
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.864 SNIP 1.805 CiteScore 2.66
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.853 SNIP 1.88 CiteScore 2.71
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.678 SNIP 1.86 CiteScore 2.47
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 2.059 SNIP 2.002 CiteScore 2.72
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 2.229 SNIP 2.145
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.502 SNIP 1.863
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 2.641 SNIP 2.04
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 2.432 SNIP 1.972
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 2.631 SNIP 2.216
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 2.773 SNIP 2.096
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 2.383 SNIP 2.238
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 2.812 SNIP 2.123
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 3.125 SNIP 2.204
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 3.635 SNIP 2.559
Web of Science (2001): Indexed yes
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Flow-structure interactions, Lubrication theory, Microfluidics
DOIs:
10.1017/jfm.2017.805
Wavelength tunable MEMS VCSELs for OCT imaging

MEMS VCSELs are one of the most promising swept source (SS) lasers for optical coherence tomography (OCT) and one of the best candidates for future integration with endoscopes, surgical probes and achieving an integrated OCT system. However, the current MEMS-based SS are processed on the III-V wafers, which are small, expensive and challenging to work with. Furthermore, the actuating part, i.e., the MEMS, is on the top of the structure which causes a strong dependence on packaging to decrease its sensitivity to the operating environment. This work addresses these design drawbacks and proposes a novel design framework. The proposed device uses a high contrast grating mirror on a Si MEMS stage as the bottom mirror, all of which is defined in an SOI wafer. The SOI wafer is then bonded to an InP III-V wafer with the desired active layers, thereby sealing the MEMS. Finally, the top mirror, a dielectric DBR (7 pairs of TiO2 - SiO2), is deposited on top. The new device is based on a silicon substrate with MEMS defined on a silicon membrane in an enclosed cavity. Thus the device is much more robust than the existing MEMS VCSELs. This design also enables either a two-way actuation on the MEMS or a smaller optical cavity (pull-away design), i.e., wider FSR (Free Spectral Range) to increase the wavelength sweep. Fabrication of the proposed device is outlined and the results of device characterization are reported.

Wavelength tunable MEMS VCSELs for OCT imaging

MEMS VCSELs are one of the most promising swept source (SS) lasers for optical coherence tomography (OCT) and one of the best candidates for future integration with endoscopes, surgical probes and achieving an integrated OCT system. However, the current MEMS-based SS are processed on the III-V wafers, which are small, expensive and challenging to work with. Furthermore, the actuating part, i.e., the MEMS, is on the top of the structure which causes a strong dependence on packaging to decrease its sensitivity to the operating environment. This work addresses these design drawbacks and proposes a novel design framework. The proposed device uses a high contrast grating mirror on a Si MEMS stage as the bottom mirror, all of which is defined in an SOI wafer. The SOI wafer is then bonded to an InP III-V wafer with the desired active layers, thereby sealing the MEMS. Finally, the top mirror, a dielectric DBR (7 pairs of TiO2 - SiO2), is deposited on top. The new device is based on a silicon substrate with MEMS defined on a silicon membrane in an enclosed cavity. Thus the device is much more robust than the existing MEMS VCSELs. This design also enables either a two-way actuation on the MEMS or a smaller optical cavity (pull-away design), i.e., wider FSR (Free Spectral Range) to increase the wavelength sweep. Fabrication of the proposed device is outlined and the results of device characterization are reported.

General information
State: Published
Organisations: Department of Photonics Engineering, Nanophotonic Devices, Nanophotonics Theory and Signal Processing, High-Speed Optical Communication, Centre of Excellence for Silicon Photonics for Optical Communications, Experimental Surface and Nanomaterials Physics, Department of Micro- and Nanotechnology, Silicon Microtechnology, OCTLIGHT ApS
Authors: Sahoo, H. K. (Intern), Ansbæk, T. (Ekstern), Ottaviano, L. (Intern), Semenova, E. (Intern), Hansen, O. (Intern), Yvind, K. (Intern)
Number of pages: 6
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Publication: Research - peer-review › Article in proceedings – Annual report year: 2018

PROCESS FOR THE PREPARATION OF ALLOY NANOPIERCLES COMPRISING A NOBLE AND A NON-NOBLE METAL
The present invention concerns a chemical process for preparing nanoparticles of an alloy comprising both a noble metal, such as platinum, and a non-noble transition or lanthanide metal, such as yttrium, gadolinium or terbium. The process is carried out by reduction with hydrogen and removal of volatile species in gas form at the reaction temperature.

General information
State: Published
Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics
Authors: Chorkendorff, I. (Intern), Stephens, I. E. L. (Ekstern), Knudsen, B. P. (Ekstern), VELAZQUEZ-PALENZUELA, A. A. (Ekstern), Pedersen, C. M. (Ekstern)
Publication date: 9 Nov 2017
HIGH PRECISION COMPUTED TOMOGRAPHY FOR METROLOGY

Disclosed is a CT system for performing measurements on an object. The CT system comprises a support element for supporting the object; a radiation source for radiating the object at a plurality of different angles; a radiation detector assembly for detecting radiation passed through the object and in response thereto generate radiation data; and a processing unit operatively connected to the radiation detector assembly. The radiation detector assembly comprises a support, a first detector array, and a second detector array, the first detector array and the second detector array being attached to the support. The processing is configured to generate tomographic images of the object by processing radiation data received from the radiation detector assembly together with first calibration data describing properties of the first detector array and second calibration data describing properties of the second detector array.

Dispersive heterodyne probing method for laser frequency stabilization based on spectral hole burning in rare-earth doped crystals

Frequency-locking a laser to a spectral hole in rare-earth doped crystals at cryogenic temperature has been shown to be a promising alternative to the use of high finesse Fabry-Perot cavities when seeking a very high short term stability laser (M. J. Thorpe et al., Nature Photonics 5, 688 (2011)). We demonstrate here a novel technique for achieving such stabilization, based on generating a heterodyne beat-note between a master laser and a slave laser whose dephasing caused by propagation near a spectral hole generate the error signal of the frequency lock. The master laser is far detuned from the center of the inhomogeneous absorption profile, and therefore exhibits only limited interaction with the crystal despite a potentially high optical power. The demodulation and frequency corrections are generated digitally with a hardware and software implementation based on a field-programmable gate array and a Software Defined Radio platform, making it straightforward to address several frequency channels (spectral holes) in parallel.
Methodology for in situ synchrotron X-ray studies in the laser-heated diamond anvil cell

A review of some important technical challenges related to in situ diamond anvil cell laser heating experimentation at synchrotron X-ray sources is presented. The problem of potential chemical reactions between the sample and the pressure medium or the carbon from the diamond anvils is illustrated in the case of elemental tantalum. Preliminary results of a comparison between reflective and refractive optics for high temperature measurements in the laser-heated diamond anvil cell are briefly discussed. Finally, the importance of the size and relative alignment of X-ray and laser beams for quantitative X-ray measurements is presented.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, European Synchrotron Radiation Facility, Commissariat a L'Energie Atomique CEA
Authors: Mezouar, M. (Ekstern), Giampaoli, R. (Ekstern), Garbarino, G. (Ekstern), Kantor, I. (Intern), Dewaele, A. (Ekstern), Weck, G. (Ekstern), Boccato, S. (Ekstern), Svitlyk, V. (Ekstern), Rosa, A. D. (Ekstern), Torchio, R. (Ekstern), Mathon, O. (Ekstern), Hignet, O. (Ekstern), Bauchau, S. (Ekstern)
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Scopus rating (2017): SNIP 0.982 SJR 0.69 CiteScore 1.62
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BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.12 SJR 0.388 SNIP 0.69
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BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.458 SNIP 0.804 CiteScore 1.08
BFI (2014): BFI-level 1
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Scopus rating (2013): SJR 0.447 SNIP 0.66 CiteScore 1.03
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
A METHOD OF SECURITY SCANNING OF CARRY-ON ITEMS, AND A CARRY-ON ITEMS SECURITY SCANNING SYSTEM

A security scanning system (1) comprises a first stage module (3) having at least one X-ray source (6) and at least three first detectors (7) that are line-shaped and arranged in mutually different orientations and have at least dual energy resolution. A group of carry-on items (4) on a carrier are scanned simultaneously in the first stage module solely by transmission contrast radiography generating projections of two-dimensional image data. A processing device (9) reconstructs a 3D representation of the carry-on items and analyzes the 3D representation to determine whether further scanning is required.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics
Authors: Poulsen, H. F. (Intern), Olsen, U. L. (Intern), Kehres, J. (Intern)
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Patent number: WO2017005757
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Priority number: EP20150175560
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**1s2p resonant inelastic X-ray scattering combined dipole and quadrupole analysis method**

In this study an analysis strategy towards using the resonant inelastic X-ray scattering (RIXS) technique more effectively compared with X-ray absorption spectroscopy (XAS) is presented. In particular, the question of when RIXS brings extra information compared with XAS is addressed. To answer this question the RIXS plane is analysed using two models: (i) an exciton model and (ii) a continuum model. The continuum model describes the dipole pre-edge excitations while the exciton model describes the quadrupole excitations. Applying our approach to the experimental 1s2p RIXS planes of VO$_2$ and TiO$_2$, it is shown that only in the case of quadrupole excitations being present is additional information gained by RIXS compared with XAS. Combining this knowledge with methods to calculate the dipole contribution in XAS measurements gives scientists the opportunity to plan more effective experiments.
Resonant inelastic X-ray scattering, RIXS, X-ray absorption, X-ray emission
Accuracy of surface strain measurements from transmission electron microscopy images of nanoparticles

Strain analysis from high-resolution transmission electron microscopy (HRTEM) images offers a convenient tool for measuring strain in materials at the atomic scale. In this paper we present a theoretical study of the precision and accuracy of surface strain measurements directly from aberration-corrected HRTEM images. We examine the influence of defocus, crystal tilt and noise, and find that absolute errors of at least 1–2% strain should be expected. The model structures include surface relaxations determined using molecular dynamics, and we show that this is important for correctly evaluating the errors introduced by image aberrations.

General information
State: Published
Organisations: Department of Physics, Theoretical Atomic-scale Physics, Center for Electron Nanoscopy
Authors: Madsen, J. (Intern), Liu, P. (Intern), Wagner, J. B. (Intern), Hansen, T. W. (Intern), Schiøtz, J. (Intern)
Number of pages: 12
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Main Research Area: Technical/natural sciences

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A combined UHV-STM-flow cell set-up for electrochemical/electrocatalytic studies of structurally well-defined UHV prepared model electrodes

We describe the construction and discuss the performance of a novel combined ultrahigh vacuum (UHV)-electrochemistry set-up, allowing the controlled preparation and structural characterization of complex nanostructured electrode surfaces by high resolution scanning tunnelling microscopy (STM) under UHV conditions on the one hand and, after electrode transfer under clean conditions, electrochemical measurements under continuous, controlled electrolyte mass transport conditions on the other. Electrochemical measurements can be coupled with online product detection, either using an additional collector electrode or by differential electrochemical mass spectrometry (DEMS). The potential of the set-up will be illustrated in two electrocatalytic reactions on complex, but structurally well-defined bimetallic electrode surfaces: O\textsubscript{2} reduction on Pt\textsubscript{x}Ag\textsubscript{1-x}/Pt(111) monolayer surface alloys and bulk CO oxidation on Pt monolayer island modified Ru(0001) electrodes. We will particularly demonstrate the importance of structural characterization after the electrochemical measurements for identifying structural modifications induced by the electrochemical environment and thus avoiding misleading conclusions about the structure-activity relationships.

General information
State: Published
Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics, National Veterinary Institute
Authors: Schnaidt, J. (Ekstern), Beckord, S. (Ekstern), Engstfeld, A. K. (Intern), Klein, J. (Intern), Brimaud, S. (Ekstern), Behm, R. J. (Ekstern)
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Main Research Area: Technical/natural sciences

Publication information
Acoustic Tweezing and Patterning of Concentration Fields in Microfluidics

We demonstrate theoretically that acoustic forces acting on inhomogeneous fluids can be used to pattern and manipulate solute concentration fields into spatiotemporally controllable configurations stabilized against gravity. A theoretical framework describing the dynamics of concentration fields that weakly perturb the fluid density and speed of sound is presented and applied to study manipulation of concentration fields in rectangular-channel acoustic eigenmodes and in Bessel-function acoustic vortices. In the first example, methods to obtain horizontal and vertical multilayer stratification of the concentration field at the end of a flow-through channel are presented. In the second example, we demonstrate acoustic tweezing and spatiotemporal manipulation of a local high-concentration region in a lower-concentration medium, thereby extending the realm of acoustic tweezing to include concentration fields.

General information

State: Published
Organisations: Department of Physics, Biophysics and Fluids
Authors: Karlsen, J. T. (Intern), Bruus, H. (Intern)
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Main Research Area: Technical/natural sciences

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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
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Æggebakken som forandringsprisme – en historie fra forbrugersamfundets fortrængte bagside

General information
A Flexible Web-Based Approach to Modeling Tandem Photocatalytic Devices

There have been several works modeling the optimal band gaps for tandem photocatalytic water splitting devices under different assumptions. Due to the many parameters involved, it is impossible for the authors to consider every conceivable situation. In this work, we have developed a web-based model (WBM) that allows users to input data such as photoabsorber diode parameters, catalytic losses, ionic losses, light concentration, etc. This program also adds a new parameter that allows one to balance the photon absorption distribution between both photoabsorbers in a tandem device (by thinning the top photoabsorber), thus allowing for a broader range of band gap combinations that can still provide highly efficient devices. While this does not change the overall maximum efficiency point, at certain band gap combinations balancing the photon absorption distribution between photoabsorbers can increase Solar to Hydrogen (STH) efficiency by up to 15% points. An additional feature of the WBM is that it allows users to upload data of a single photoelectrode, and then investigate the optimal matching photoabsorber band gap to maximize tandem device efficiency. This work analyzes some of the best previous experimental photoelectrodes, and quantitatively relates their performance to what would typically be expected via modeling programs.
Alloy design as an inverse problem of cluster expansion models

Central to a lattice model of an alloy system is the description of the energy of a given atomic configuration, which can be conveniently developed through a cluster expansion. Given a specific cluster expansion, the ground state of the lattice model at 0 K can be solved by finding the configuration of solutes that minimizes the energy of the system. In this paper, we develop a method for solving the inverse lattice problem, where, given a broad class of potential, we find the ground states for all possible values of the effective cluster interaction energies. To do so, we formulate the inverse problem in terms of energetically distinct configurations, using a constraint satisfaction model to identify constructible configurations, and show that a convex hull can be used to identify ground states. To demonstrate the approach, we solve for all ground states for a binary alloy in a 2D hexagonal lattice both with and without an interface, based on pairwise interactions.
A low-spin Fe(III) complex with 100-ps ligand-to-metal charge transfer photoluminescence

Transition-metal complexes are used as photosensitizers(1), in light-emitting diodes, for biosensing and in photocatalysis(2). A key feature in these applications is excitation from the ground state to a charge-transfer state(3,4); the long charge-transfer-state lifetimes typical for complexes of ruthenium(5) and other precious metals are often essential to ensure high performance. There is much interest in replacing these scarce elements with Earth-abundant metals, with iron(6) and copper(7) being particularly attractive owing to their low cost and non-toxicity. But despite the exploration of innovative molecular designs(6,8-10), it remains a formidable scientific challenge(11) to access Earth-abundant transition-metal complexes with long-lived charge-transfer excited states. No known iron complexes are considered(12) photoluminescent at room temperature, and their rapid excited-state deactivation precludes their use as photosensitizers(13-15). Here we present the iron complex \([\text{Fe(btz)}(3)]^{3+}\) (where btz is 3,3'-dimethyl-1,1'-bis(p-tolyl)-4,4'-bis(1,2,3-triazol-5-ylidene)), and show that the superior sigma-donor and pi-acceptor electron properties of the ligand stabilize the excited state sufficiently to realize a long charge-transfer lifetime of 100 picoseconds (ps) and room-temperature photoluminescence. This species is a low-spin Fe(III) d(5) complex, and emission occurs from a long-lived doublet ligand-to-metal charge-transfer ((LMCT)-L-2) state that is rarely seen for transition-metal complexes(4,16,17). The absence of intersystem crossing, which often gives rise to large excited-state energy losses in transition-metal complexes, enables the observation of spin-allowed emission directly to the ground state and could be exploited as an increased driving force in photochemical reactions on surfaces. These findings suggest that appropriate design strategies can deliver new iron-based materials for use as light emitters and photosensitizers.

General information
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Organisations: Neutrons and X-rays for Materials Physics, Department of Physics, Lund University, Uppsala University, University of Copenhagen, National Institute of Standards and Technology
Ammonia synthesis from N\textsubscript{2} and H\textsubscript{2}O using a lithium cycling electrification strategy at atmospheric pressure

Ammonia production is imperative to providing food for a growing world population. However, the primary method of synthetic ammonia production, the Haber Bosch process, is resource demanding and unsustainable. Here we report a novel ammonia production strategy, exemplified in an electrochemical lithium cycling process, which provides a pathway to sustainable ammonia synthesis via the ability to directly couple to renewable sources of electricity and can facilitate localized production. Whereas traditional aqueous electrochemical approaches are typically dominated by the hydrogen evolution reaction (HER), we are able to circumvent the HER by using a stepwise approach which separates the reduction of N\textsubscript{2} from subsequent protonation to NH\textsubscript{3}, thus our synthesis method is predominantly selective for ammonia production. Density functional theory calculations for thermodynamic and diffusion energy barrier insights suggest that Li-based materials are well suited to carry out this process, though other materials may also be useful. The three steps of the demonstrated process are LiOH electrolysis, direct nitridation of Li, and the exothermic release of ammonia from Li\textsubscript{3}N, which reproduces the LiOH, completing the cycle. The process uses N\textsubscript{2} and H\textsubscript{2}O at atmospheric pressure and reasonable temperatures, and, while approaching industrial level electrolytic current densities, we report an initial current efficiency of 88.5% toward ammonia production.

General information
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Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics, Stanford University
Authors: McEnaney, J. M. (Ekstern), Singh, A. R. (Ekstern), Schwalbe, J. A. (Ekstern), Kibsgaard, J. (Intern), Lin, J. C. (Ekstern), Cargnello, M. (Ekstern), Jaramillo, T. F. (Ekstern), Norskov, J. K. (Ekstern)
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Main Research Area: Technical/natural sciences
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Web of Science (2017): Indexed yes
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Scopus rating (2016): CiteScore 26.39 SJR 12.283 SNIP 4.325
A Monte Carlo simulation of scattering reduction in spectral x-ray computed tomography

In X-ray computed tomography (CT), scattered radiation plays an important role in the accurate reconstruction of the inspected object, leading to a loss of contrast between the different materials in the reconstruction volume and cupping artifacts in the images. We present a Monte Carlo simulation tool for spectral X-ray CT to predict the scattered radiation generated by complex samples. An experimental setup is presented to isolate the energy distribution of scattered radiation. Spectral CT is a novel technique implementing photon-counting detectors able to discriminate the energy of incoming photons, enabling spectral analysis of X-ray images. This technique is useful to extract efficiently more information on energy dependent quantities (e.g. mass attenuations coefficients) and study matter interactions (e.g. X-ray scattering, photoelectric absorption, etc...). Having a good knowledge of the spectral distribution of the scattered X-rays is fundamental to establish methods attempting to correct for it. The simulations are validated by real measurements using a CdTe spectral resolving detector (Multix ME-100). We observed the effect of the scattered radiation on the image reconstruction, becoming relevant in the energy range where the Compton events are dominant (i.e. above 50keV).

General information

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Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Department of Applied Mathematics and Computer Science, Image Analysis & Computer Graphics, National Space Institute, Niels Bohr Institute
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Article number: 103880P
An analytical model of flagellate hydrodynamics

Flagellates are unicellular microswimmers that propel themselves using one or several beating flagella. We consider a hydrodynamic model of flagellates and explore the effect of flagellar arrangement and beat pattern on swimming kinematics and near-cell flow. The model is based on the analytical solution by Oseen for the low Reynolds number flow due to a point force outside a no-slip sphere. The no-slip sphere represents the cell and the point force a single flagellum. By superposition we are able to model a freely swimming flagellate with several flagella. For biflagellates with left–right symmetric flagellar arrangements we determine the swimming velocity, and we show that transversal forces due to the periodic movements of the flagella can promote swimming. For a model flagellate with both a longitudinal and a transversal flagellum we determine radius and pitch of the helical swimming trajectory. We find that the longitudinal flagellum is responsible for the average translational motion whereas the transversal flagellum governs the rotational motion. Finally, we show that the transversal flagellum can lead to strong feeding currents to localized capture sites on the cell surface.
Solid oxide oxygen ion and proton conductors are a highly important class of materials for renewable energy conversion devices like solid oxide fuel cells. $\text{Ba}_2\text{In}_2\text{O}_5$ (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.
Assessing the performance of the random phase approximation for exchange and superexchange coupling constants in magnetic crystalline solids

The random phase approximation (RPA) for total energies has previously been shown to provide a qualitatively correct description of static correlation in molecular systems, where density functional theory (DFT) with local functionals are bound to fail. This immediately poses the question of whether the RPA is also able to capture the correct physics of strongly correlated solids such as Mott insulators. Due to strong electron localization, magnetic interactions in such systems are dominated by superexchange, which in the simplest picture can be regarded as the analog of static correlation for molecules. In this paper, we investigate the performance of the RPA for evaluating both superexchange and direct exchange interactions in the magnetic solids NiO, MnO, Na₃Cu₂SbO₆, Sr₂CuO₃, Sr₂CuTeO₆, and a monolayer of CrI₃, which were chosen to represent a broad variety of magnetic interactions. It is found that the RPA can accurately correct the large errors introduced by Hartree-Fock, independent of the input orbitals used for the perturbative expansion. However, in most cases, accuracies similar to RPA can be obtained with DFT+U, which is significantly simpler from a computational point of view.
A Strategy to Suppress Phonon Transport in Molecular Junctions Using pi-Stacked Systems

Molecular junctions are promising candidates for thermoelectric devices due to the potential to tune the electronic and thermal transport properties. However, a high figure of merit is hard to achieve, without reducing the phononic contribution to thermal conductance. Here, we propose a strategy to suppress phonon transport in graphene-based molecular junctions preserving high electronic power factor, using nonbonded pi-stackal systems. Using first-principles calculations, we find that the thermal conductance of pi-stackd systems can be reduced by about 95%, compared with that of a covalently bonded molecular junction. Phonon transmission of pi-stacked systems is largely attenuated in the whole frequency range, and the remaining transmission occurs mainly below 5 THz, where out-of-plane channels dominate. The figure of merit (ZT) of the pi-stacked molecular junction is dramatically enhanced because of the very low phononic thermal conductance, leaving tom for further optimization of the electronic properties.
A Study of Deactivating Carbon Species during Methanation on a Ni/Al₂O₃ Catalyst

This Ph.D. thesis describes the research and findings from experimental testing of a methanation catalyst and the characterisation of said catalyst. Methanation is the conversion of syngas (CO and H₂) typically from coal or biomass to methane and water. Methane is the biggest constituent of natural gas and as the infrastructure is already in place for natural gas, it is an attractive alternative to depleting oil resources. Catalysts based on nickel are the most common choice within industry due to the relatively low price of nickel and its acceptable performance. However, nickel catalysts are prone to deactivate due to sintering and carbon deposition. The latter process is not well understood and thus, this work attempted to further the research in low temperature carbon formation. In order to obtain fundamental knowledge, the experimental setup had to be free of impurities and great care was taken to eliminate potential sources. Experiments designed for that purpose established that the influence of sulfur was negligible. Through a series of experiments of temperature programmed hydrogenation (TPH) - methanation - TPH, the carbon build-up during the methanation was studied by the second TPH. Four types of carbon were identified and especially one was found to be the main cause of deactivation. Through X-ray diffraction (XRD) it was established that part of the carbon dissolved into the nickel particles expanding the crystal structure. No carbon was observed during transmission electron microscopy (TEM). Yet by scanning transmission electron microscopy (STEM) energy dispersive spectroscopy (EDS) carbon was discovered in proximity to the nickel particles. However, this was not as well-defined shells and thus, it was deduced that the particles were not encapsulated by carbon. Instead, the carbon was likely very inhomogeneously distributed across the nickel surface, which was supported by remaining activity observed during the methanation tests. Preliminary results on the effect of particle size, temperature and total pressure of methanation showed that especially temperature greatly affected the types of carbon deposited.

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Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics
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Autoresonant control of drift waves

The control of nonlinear drift waves in a magnetized plasmas column has been investigated. The studies are based on the Hasegawa–Mima model, which is solved on a disk domain with radial inhomogeneity of the plasma density. The system is forced by a rotating potential with varying frequency defined on the boundary. To excite and control the waves we apply the autoresonant effect, taking place when the amplitude of the forcing exceeds a threshold value and the waves are phase-locked with the forcing. We demonstrate that the autoresonant approach is applicable for excitation of a range of steady nonlinear waves of the lowest azimuthal mode numbers and for controlling their amplitudes and phases. We also demonstrate the excitation of zonal flows ($m = 0$ modes), which are controlled via the forced modes.
Band structure engineered layered metals for low-loss plasmonics

Plasmonics currently faces the problem of seemingly inevitable optical losses occurring in the metallic components that challenges the implementation of essentially any application. In this work, we show that Ohmic losses are reduced in certain layered metals, such as the transition metal dichalcogenide TaS2, due to an extraordinarily small density of states for scattering in the near-IR originating from their special electronic band structure. On the basis of this observation, we propose a new class of band structure engineered van der Waals layered metals composed of hexagonal transition metal chalcogenide-halide layers with greatly suppressed intrinsic losses. Using first-principles calculations, we show that the suppression of optical losses lead to improved performance for thin-film waveguiding and transformation optics.

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Organisations: Center for Nanostructured Graphene, Department of Physics, Theoretical Atomic-scale Physics
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Band structure engineering in van der Waals heterostructures via dielectric screening: the GΔW method

The idea of combining different two-dimensional (2D) crystals in van der Waals heterostructures (vdWHs) has led to a new paradigm for band structure engineering with atomic precision. Due to the weak interlayer couplings, the band structures of the individual 2D crystals are largely preserved upon formation of the heterostructure. However, regardless of the details of the interlayer hybridisation, the size of the 2D crystal band gaps are always reduced due to the enhanced dielectric screening provided by the surrounding layers. The effect can be significant (on the order of electron volts) but its precise magnitude is non-trivial to predict because of the non-local nature of the screening in quasi-2D crystals. Moreover, the effect is not captured by effective single-particle methods such as density functional theory. Here we present an efficient and general method for calculating the band gap renormalization of a 2D material embedded in an arbitrary vdWH. The method evaluates the change in the GW self-energy of the 2D material from the change in the screened Coulomb interaction. The latter is obtained using the quantum-electrostatic heterostructure (QEH) model. We benchmark the GΔW method against full first-principles GW calculations and use it to unravel the importance of screening-induced band structure renormalisation in various vdWHs. A main result is the observation that the size of the band gap reduction of a given 2D material when inserted into a heterostructure scales inversely with the polarisability of the 2D material. Our work demonstrates that dielectric engineering via van der Waals heterostructuring represents a promising strategy for tailoring the band structure of 2D materials.

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Web of Science (2017): Indexed yes
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Beamstop-based low-background ptychography to image weakly scattering objects

In recent years, X-ray ptychography has been established as a valuable tool for high-resolution imaging. Nevertheless, the spatial resolution and sensitivity in coherent diffraction imaging are limited by the signal that is detected over noise and over background scattering. Especially, coherent imaging of weakly scattering specimens suffers from incoherent background that is generated by the interaction of the central beam with matter along its propagation path in particular close to and inside of the detector. Common countermeasures entail evacuated flight tubes or detector-side beamstops, which improve the experimental setup in terms of background reduction or better coverage of high dynamic range in the diffraction patterns. Here, we discuss an alternative approach: we combine two ptychographic scans with and without beamstop and reconstruct them simultaneously taking advantage of the complementary information contained in the two scans. We experimentally demonstrate the potential of this scheme for hard X-ray ptychography by imaging a weakly scattering object composed of catalytic nanoparticles and provide the analysis of the signal-to-background ratio in the diffraction patterns.

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Organisations: Department of Physics, Center for Electron Nanoscopy, Experimental Surface and Nanomaterials Physics, Department of Chemical and Biochemical Engineering, Deutsches Elektronensynchrotron DESY, Technische Universität Dresden, Karlsruhe Institute of Technology KIT
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Scopus rating (2014): SJR 1.628 SNIP 1.598 CiteScore 2.59
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Benchmarking Pt and Pt-lanthanide sputtered thin films for oxygen electroreduction: fabrication and rotating disk electrode measurements

Platinum-lanthanide alloys are very promising as active and stable catalysts for the oxygen reduction reaction (ORR) in low-temperature fuel cells. We have fabricated Pt and Pt$_5$Gd metallic thin films via (co-)sputtering deposition in an ultra-high vacuum (UHV) chamber. The electrochemical ORR activity, stability, as well as chemical composition and crystallographic structure of Pt$_5$Gd thin film catalysts have been investigated using a combination of electrochemical measurements, X-ray photoemission spectroscopy (XPS) and X-ray diffraction (XRD) techniques. We describe the measurement procedures, with the aim of benchmarking electrochemical characterization of Pt-based thin film catalysts for ORR. Pt$_5$Gd thin films present an activity enhancement by a factor of 4.5 and 2.5 over polycrystalline Pt and Pt thin films, respectively.

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Boosting the Open Circuit Voltage of Cu$_2$ZnSnS$_4$ Solar Cells by a Lattice-Matched CeO$_2$ Layer and Theoretical Understanding of Interface Defects

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Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics, Silicon Microtechnology, Department of Micro- and Nanotechnology, Theoretical Nanoelectronics, Department of Photonics Engineering, Optical Microsensors and Micromaterials, University of New South Wales, QuantumWise A/S
Authors: Crovetto, A. (Intern), Yan, C. (Ekstern), Palsgaard, M. L. N. (Intern), Iandolo, B. (Intern), Zhou, F. (Ekstern), Gunst, T. (Intern), Markussen, T. (Ekstern), Stride, J. (Ekstern), Schou, J. (Intern), Stokbro, K. (Ekstern), Brandbyge, M. (Intern), Hao, X. (Ekstern), Hansen, O. (Intern)
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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 CuRu catalyst is attributed to changes in the electronic structure, and thus the altered adsorption properties of the surface Cu sites.
Bounds on the stably recoverable information for the Helmholtz equation in $\mathbb{R}^2$

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Buen og gnisten
Anmeldelse af Lise Bock "Buen og gnisten. Pionererne fra radioens barndom"

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Calculating excitons, plasmons, and quasiparticles in 2D materials and van der Waals heterostructures: Topical Review

Atomically thin two-dimensional (2D) materials host a rich set of electronic states that differ substantially from those of their bulk counterparts due to quantum confinement and enhanced many-body effects. This Topical Review focuses on the theory and computation of excitons, plasmons and quasiparticle band structures in 2D materials and their heterostructures. The general theory is illustrated by applications to various types of 2D materials including transition metal dichalcogenides, graphene, phosphorene, and hexagonal boron nitride. The weak and highly non-local dielectric function of atomically thin crystals is shown to be responsible for many of the unique properties exhibited by the 2D materials such as the formation of strongly bound, non-Hydrogenic excitons, large band gap renormalization effects, and the different signatures of excitons and plasmons in electron energy loss spectroscopy (EELS). Among other topics covered are spin-orbit coupling, trions, interlayer excitons, exciton dissociation, and environmental screening. Technical issues associated with the application of the many-body GW method and the Bethe-Salpeter equation (BSE) to 2D materials are also discussed. A combined quantum/classical method is introduced and used throughout to account for dielectric screening and self-energy effects from substrates and van der Waals heterostructures including the difficult case of non-matching lattices.
Carrier-selective p- and n-contacts for efficient and stable photocatalytic water reduction

The successful realization of carrier-selective contacts for crystalline silicon (c-Si) based device for photocatalytic hydrogen production has been demonstrated. The proposed TiO₂-protected carrier-selective contacts resemble a metal-oxide-semiconductor configuration, including a highly-doped nanocrystalline silicon (nc-Si) and a tunnel oxide, thereby forming a heterostructure with the c-Si substrate. By substituting conventional pn+-junction Si by c-Si/SiOₓ/nc-Si structure for both front and back contacts we demonstrate a 16% increase in photovoltage (an open circuit voltage of 584 mV under AM 1.5G conditions). TiO₂ protected carrier-selective photoelectrodes showed excellent long-term durability in acidic aqueous solution having stable photocurrent output for more than 40 days, implying that the proposed carrier-selective contact is a promising configuration to substitute for the conventional pn-junction based c-Si photocathodes.
Cascades of alternating pitchfork and flip bifurcations in H-bridge inverters

Power electronic DC/AC converters (inverters) play an important role in modern power engineering. These systems are also of considerable theoretical interest because their dynamics is influenced by the presence of two vastly different forcing frequencies. As a consequence, inverter systems may be modeled in terms of piecewise smooth maps with an extremely high number of switching manifolds. We have recently shown that models of this type can demonstrate a complicated bifurcation structure associated with the occurrence of border collisions. Considering the example of a PWM H-bridge single-phase inverter, the present paper discusses a number of unusual phenomena that can occur in piecewise smooth maps with a very large number of switching manifolds. We show in particular how smooth (pitchfork and flip) bifurcations may form a macroscopic pattern that stretches across the overall bifurcation structure. We explain the observed bifurcation phenomena, show under which conditions they occur, and describe them quantitatively by means of an analytic approximation.

General information
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Organisations: Department of Physics, University of Stuttgart, Southwest State University
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Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.847 SNIP 1.211 CiteScore 1.71
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Scopus rating (2008): SJR 1.692 SNIP 1.533
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.595 SNIP 1.594
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.512 SNIP 1.346
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.632 SNIP 1.739
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.686 SNIP 1.831
Scopus rating (2003): SJR 1.868 SNIP 1.781
Scopus rating (2002): SJR 1.646 SNIP 1.531
Scopus rating (2001): SJR 1.859 SNIP 1.683
Scopus rating (2000): SJR 1.215 SNIP 1.545
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Challenges in bimetallic multilayer structure formation: Pt growth on Cu monolayers on Ru(0001)

In a joint experimental and theoretical study, we investigated the formation and morphology of PtCu/Ru(0001) bimetallic surfaces grown at room and higher temperatures under UHV conditions. We obtained the PtCu/Ru(0001) surfaces by deposition of Pt atoms on a previously created Cu/Ru(0001) structure which includes only one Cu monolayer. Bimetallic surfaces prepared at different Pt coverages are investigated using STM imaging, revealing the existence of reconstruction lines and Cu islands. Although primarily created Cu islands continue growing in size by increasing Pt coverage, a continuous formation of new Cu islands is observed. This leads to an atypical exponential increase of the island density as
well as to an atypical behavior of the average number of atoms per island for low Pt coverages. Although coalescence of the islands is observed for high Pt coverages, the island density remains almost constant in that regime. In order to understand the trends observed in the experiments, we study the stability of these surfaces, atom adsorption, and adatom diffusion using periodic density functional theory calculations. On the basis of the experimental observations and the first-principles calculations, we suggest a model that includes exchange of Pt adatoms with Cu surface atoms, Pt and Cu adatom diffusion, and attractive (repulsive) interactions between Cu (Pt) adatoms with substitutional Pt surface atoms, which explains the main trends in island formation and growth observed in the experiment.

General information
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Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics
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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
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ISI indexed (2013): ISI indexed yes
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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
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Coexistence between silent and bursting states in a biophysical Hodgkin-Huxley-type of model
Classification of the dynamical mechanisms that support bistability between bursting oscillations and silence has not yet been clarified in detail. The purpose of this paper is to demonstrate that the coexistence of a stable equilibrium point with a state of continuous bursting can occur in a slightly modified, biophysical model that describe the dynamics of pancreatic beta-cells. To realize this form of coexistence, we have introduced an additional voltage-dependent potassium current that is activated in the region around the original, unstable equilibrium point. It is interesting to note that this modification also leads the model to display a blue-sky catastrophe in the transition region between chaotic and bursting states.

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Scopus rating (2017): CiteScore 2.07 SJR 0.716 SNIP 0.829
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 1.76 SJR 0.78 SNIP 0.943
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.829 SNIP 1.005 CiteScore 1.76
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Coherent structural trapping through wave packet dispersion during photoinduced spin state switching

The description of ultrafast nonadiabatic chemical dynamics during molecular photo-transformations remains challenging because electronic and nuclear configurations impact each other and cannot be treated independently. Here we gain experimental insights, beyond the Born-Oppenheimer approximation, into the light-induced spin-state trapping dynamics of the prototypical [Fe(bpy)$_3$]$^{2+}$ compound by time-resolved X-ray absorption spectroscopy at sub-30-femtosecond resolution and high signal-to-noise ratio. The electronic decay from the initial optically excited electronic state towards the high spin state is distinguished from the structural trapping dynamics, which launches a coherent oscillating wave packet (265 fs period), clearly identified as molecular breathing. Throughout the structural trapping, the dispersion of the wave packet along the reaction coordinate reveals details of intramolecular vibronic coupling before a slower vibrational energy dissipation to the solution environment. These findings illustrate how modern time-resolved X-ray absorption spectroscopy can provide key information to unravel dynamic details of photo-functional molecules.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, SLAC National Accelerator Laboratory, Laboratori Nazionali di Frascati, University of Bordeaux, University of Rennes
Authors: Lemke, H. T. (Ekstern), Kjær, K. S. (Intern), Hartsock, R. (Ekstern), Brandt van Driel, T. (Intern), Chollet, M. (Ekstern), Glownia, J. M. (Ekstern), Song, S. (Ekstern), Zhu, D. (Ekstern), Pace, E. (Ekstern), Matar, S. F. (Ekstern),
Collective Thomson scattering data analysis for Wendelstein 7-X

Collective Thomson scattering (CTS) diagnostic is being installed on the Wendelstein 7-X stellarator to measure the bulk ion temperature in the upcoming experimental campaign. In order to prepare for the data analysis, a forward model of the diagnostic (eCTS) has been developed and integrated into the Bayesian data analysis framework Minerva. Synthetic spectra have been calculated with the forward model and inverted using Minerva in order to demonstrate the feasibility to measure the ion temperature in the presence of nuisance parameters that also influence CTS spectra. In this paper we report on the results of this analysis and discuss the main sources of uncertainty in the CTS data analysis.
Colloidal Flower-Shaped Iron Oxide Nanoparticles: Synthesis Strategies and Coatings

The assembly of magnetic cores into regular structures may notably influence the properties displayed by a magnetic colloid. In this work, key synthesis parameters driving the self-assembly process capable of organizing colloidal magnetic cores into highly regular and reproducible multi-core nanoparticles are determined. In addition, a self-consistent picture that explains the collective magnetic properties exhibited by these complex assemblies is achieved through structural,
colloidal, and magnetic means. For this purpose, different strategies to obtain flower-shaped iron oxide assemblies in the size range 25–100 nm are examined. The routes are based on the partial oxidation of Fe(OH)$_2$, polyol-mediated synthesis or the reduction of iron acetylacetonate. The nanoparticles are functionalized either with dextran, citric acid, or alternatively embedded in polystyrene and their long-term stability is assessed. The core size is measured, calculated, and modeled using both structural and magnetic means while the Debye model and multi-core extended model are used to study interparticle interactions. This is the first step toward standardized protocols of synthesis and characterization of flower-shaped nanoparticles.

**General information**

**State:** Published

**Organisations:** Department of Physics, Neutrons and X-rays for Materials Physics, Department of Micro- and Nanotechnology, Magnetic Systems, Universidad Complutense, Micromod Partikeltechnologie GmbH, nanoPET Pharma GmbH, SP Technical Research Institute of Sweden, UCL Healthcare Biomagnetics Laboratory, Physikalisch-Technische Bundesanstalt, Chalmers University of Technology, University of Cantabria, Technische Universität Braunschweig, Uppsala University


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

**Publication information**

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BFI (2017): BFI-level 1

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Web of Science (2017): Indexed Yes

BFI (2016): BFI-level 1

Scopus rating (2016): CiteScore 4.01 SJR 1.468 SNIP 0.792

BFI (2015): BFI-level 1

Scopus rating (2015): SJR 1.35 SNIP 0.793 CiteScore 3.85

BFI (2014): BFI-level 1

Scopus rating (2014): SJR 0.996 SNIP 0.556 CiteScore 2.7

BFI (2013): BFI-level 1

Scopus rating (2013): SJR 0.231 SNIP 0.323 CiteScore 0.6

BFI (2012): BFI-level 1

Scopus rating (2012): SJR 0.272 SNIP 1.039 CiteScore 0.96

BFI (2011): BFI-level 1

Scopus rating (2011): SJR 0.251 SNIP 0.741 CiteScore 0.77

BFI (2010): BFI-level 1

Scopus rating (2010): SJR 0.358 SNIP 0.761

BFI (2009): BFI-level 1

Scopus rating (2009): SJR 0.404 SNIP 0.638

BFI (2008): BFI-level 1

Scopus rating (2008): SJR 0.393 SNIP 0.55

Scopus rating (2007): SJR 0.321 SNIP 0.678

Scopus rating (2006): SJR 0.426 SNIP 1.101

Scopus rating (2005): SJR 0.643 SNIP 1.097

Scopus rating (2004): SJR 0.385 SNIP 0.764

Scopus rating (2003): SJR 0.466 SNIP 0.885

Scopus rating (2002): SJR 0.205 SNIP 0.644
Combining theory and experiment in electrocatalysis: Insights into materials design

Electrocatalysis plays a central role in clean energy conversion, enabling a number of sustainable processes for future technologies. This review discusses design strategies for state-of-the-art heterogeneous electrocatalysts and associated materials for several different electrochemical transformations involving water, hydrogen, and oxygen, using theory as a means to rationalize catalyst performance. By examining the common principles that govern catalysis for different electrochemical reactions, we describe a systematic framework that clarifies trends in catalyzing these reactions, serving as a guide to new catalyst development while highlighting key gaps that need to be addressed. We conclude by extending this framework to emerging clean energy reactions such as hydrogen peroxide production, carbon dioxide reduction, and nitrogen reduction, where the development of improved catalysts could allow for the sustainable production of a broad range of fuels and chemicals.

General information
State: Published
Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics, Stanford University
Authors: Seh, Z. W. (Ekstern), Kibsgaard, J. (Intern), Dickens, C. F. (Ekstern), Chorkendorff, I. (Intern), Nørskov, J. K. (Ekstern), Jaramillo, T. F. (Ekstern)
Number of pages: 12
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Science
Volume: 355
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Web of Science (2018): Indexed yes
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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
Combining X-ray and Electron Based in situ Characterization of Catalysts

General information
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Organisations: Center for Electron Nanoscopy, Department of Physics, Experimental Surface and Nanomaterials Physics
Authors: Damsgaard, C. D. (Intern)
Number of pages: 2
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Event: Abstract from Combining electrons with X-rays for integrated in-operando experiments, trieste, Italy.
Main Research Area: Technical/natural sciences
Electronic versions:

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Activities:
Combining X-ray and Electron Based in situ Characterization of Catalysts
Source: PublicationPreSubmission
Source-ID: 137265380
Comment on "Active sites for CO₂ hydrogenation to methanol on Cu/ZnO catalyts"

Kattel et al (Reports, 24 March 2017, p. 1296) report that a zinc on copper (Zn/Cu) surface undergoes oxidation to zinc oxide/copper (ZnO/Cu) during carbon dioxide (CO₂) hydrogenation to methanol and conclude that the Cu-ZnO interface is the active site for methanol synthesis. Similar experiments conducted two decades ago by Fujitani and Nakamura et al demonstrated that Zn is attached to formate rather than being fully oxidized.

General information
State: Published
Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics, University of Tsukuba, National Institute of Advanced Industrial Science and Technology, Haldor Topsoe AS
Authors: Nakamura, J. (Ekstern), Fujitani, T. (Ekstern), Kuld, S. (Ekstern), Helveg, S. (Ekstern), Chorkendorff, I. (Intern), Sehested, J. (Ekstern)
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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
Complex band structure and electronic transmission eigenchannels

It is natural to characterize materials in transport junctions by their conductance length dependence, beta. Theoretical estimations of beta are made employing two primary theories: complex band structure and density functional theory (DFT) Landauer transport. It has previously been shown that the beta value derived from total Landauer transmission can be related to the beta value from the smallest vertical bar k(i)vertical bar complex band; however, it is an open question whether there is a deeper relationship between the two. Here we probe the details of the relationship between transmission and complex band structure, in this case individual eigenchannel transmissions and different complex bands. We present calculations of decay constants for the two most conductive states as determined by complex band structure and standard DFT Landauer transport calculations for one semiconductor and two molecular junctions. The molecular junctions show that both the length dependence of the total transmission and the individual transmission eigenvalues can be, almost always, found through the complex band structure. The complex band structure of the semi-conducting material, however, does not predict the length dependence of the total transmission but only of the individual channels, at some k-points, due to multiple channels contributing to transmission. We also observe instances of vertical bands, some of which are the smallest vertical bar k(i)vertical bar complex bands, that do not contribute to transport. By understanding the deeper relationship between complex bands and individual transmission eigenchannels, we can make a general statement about when the previously accepted wisdom linking transmission and complex band structure will fail, namely, when multiple channels contribute significantly to the transmission. Published by AIP Publishing.
Computational Fluid Dynamics of Choanoflagellate Filter-Feeding

Choanoflagellates are unicellular aquatic organisms with a single flagellum that drives a feeding current through a funnel-shaped collar filter on which bacteria-sized prey are caught. Using computational fluid dynamics (CFD) we model the beating flagellum and the complex filter flow of the choanoflagellate Diaphanoeca grandis. Our CFD simulations based on the current understanding of the morphology underestimate the experimentally observed clearance rate by more than an order of magnitude: The beating flagellum is simply unable to draw enough water through the fine filter. Our observations motivate us to suggest a radically different filtration mechanism that requires a flagellar vane (sheet), and addition of a wide vane in our CFD model allows us to correctly predict the observed clearance rate.

General information
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Organisations: Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering, National Institute of Aquatic Resources, Centre for Ocean Life, Department of Physics, Biophysics and Fluids
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Main Research Area: Technical/natural sciences
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Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2017

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
Computational screening of new inorganic materials for highly efficient solar energy conversion

The world’s energy consumption is rising, and the demand for energy is projected to increase even more in the future. At the moment, we rely on energy from fossil fuels, which are harmful to the environment, and the future increases in consumption will be strongly harmful to both the environment and human well being. Additionally, fossil fuels are non-renewable, and there are only limited reserves on the planet. An alternative to using fossil fuels is to harvest energy from renewable and environmentally benign sources, such as the sun, which theoretically provides the largest source of energy that we have access to. Despite the vast amounts of energy at our disposal, we are not able to harvest this solar energy efficiently. Currently, there are a few ways of converting solar power into usable energy, such as photovoltaics (PV) or photoelectrochemical generation of fuels (PC). PV processes in solar cells convert solar energy into electricity, and PC uses harvested energy to conduct chemical reactions, such as splitting water into oxygen and, more importantly, hydrogen, also known as the fuel of the future.

Further progress in both PV and PC fields is mostly limited by the flaws in materials used as photoabsorbers. Silicon as an absorber dominantes the PV community and all other semiconductors face significant challenges, for various different reasons, when suggested for large scale deployment. Advances in PC, on the other hand, are mostly held back due to the fact that no single material, which can both absorb light and catalyse the relevant chemical reactions, has been found. A proposed alternative, using two materials in tandem instead of one, has the potential to successfully perform the task. However, progress in this field is inhibited by the lack of high band gap photoabsorbing materials. In this work a high-throughput computational search for suitable absorbers for PV and PC applications is presented. A set of descriptors has been developed, such that each descriptor targets an important property or issue of a good solar energy conversion material. The screening study was performed step-wise, so that in each step a new descriptor and associated criterion were introduced and all the materials failing to satisfy the criterion are removed from the study. The corresponding descriptors were obtained within the scope of quantum mechanics using Density Functional Theory. One of these candidates has been successfully synthesized by our collaborators, and the measured band gap is in accordance with the theoretically calculated one. Furthermore, a study on previously synthesized semiconductors yielded a list of stable materials which have not yet been explored for PV or PC.

A similar study has been performed on II-IV-V2 compounds, and has revealed some interesting trends within the class, resulting in several interesting candidate materials. A few of these have already been extensively investigated by others.
Conceptual design of the Radial Gamma Ray Spectrometers system for α particle and runaway electron measurements at ITER

We here present the principles and main physics capabilities behind the design of the radial gamma ray spectrometers (RGRS) system for alpha particle and runaway electron measurements at ITER. The diagnostic benefits from recent advances in gamma-ray spectrometry for tokamak plasmas and combines space and high energy resolution in a single device. The RGRS system as designed can provide information on α particles on a time scale of 1/10 of the slowing down time for the ITER 500 MW full power DT scenario. Spectral observations of the 3.21 and 4.44 MeV peaks from the $^9$Be$(\alpha, n\gamma)$ $^{12}$C reaction make the measurements sensitive to α particles at characteristic resonant energies and to possible anisotropies of their slowing down distribution function. An independent assessment of the neutron rate by gamma-ray emission is also feasible. In case of runaway electrons born in disruptions with a typical duration of 100ms, a time resolution of at least 10ms for runaway electron studies can be achieved depending on the scenario and down to a current of 40 kA by use of external gas injection. We find that the bremsstrahlung spectrum in the MeV range from confined runaways is sensitive to the electron velocity space up to $E \approx 30$–40 MeV, which allows for measurements of the energy distribution of the runaway electrons at ITER.
Correction to: Accuracy of surface strain measurements from transmission electron microscopy images of nanoparticles

Unfortunately, after publication of this article [1], it was noticed that the name of the fifth author was incorrectly displayed as Jakob Schiøz. The correct name is Jakob Schiøtz and can be seen in the corrected author list above. The original article has also been updated to correct this error.

General information
State: Published
Organisations: Department of Physics, Theoretical Atomic-scale Physics, Center for Electron Nanoscopy
Authors: Madsen, J. (Intern), Liu, P. (Intern), Wagner, J. B. (Intern), Hansen, T. W. (Intern), Schiøtz, J. (Intern)
Number of pages: 12
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Main Research Area: Technical/natural sciences

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Volume: 3
Issue number: 1
ISSN (Print): 2198-0926
Ratings:
Crack Tip Flipping under Mode I Tearing: Investigated by X-Ray Tomography

The fracture surface morphology that results from mode I tearing of ductile plate metals depends heavily on both the elastic-plastic material properties and the microstructure. Severe tunneling of the advancing crack tip (resulting in cup-cup, or bath-tub like fracture surfaces) can take place in a range of materials, often of low strength, while tearing of high strength metals typically progress by the shear band failure mechanism (slanting). In reality, however, most fracture surfaces display a mixture of morphologies. For example, slant crack propagation can be accompanied by large shear lips near the outer free plate surface or a complete shear band switch − seemingly distributed randomly on the fracture surface. The occasionally observed shear band switch of mode I slant cracks, related to ductile plate tearing, is far from random as the crack can flip systematically from one side to the other in roughly 45-degree shear bands. This "flipping" action of a slanted crack remains to be fully understood, and the present study serves to share details on the phenomenon by exploiting X-ray tomography scanning to access the plate interior and the very crack tip. Throughout, the focus is on a crack tip where the flip is underway. Extensive growth of single edge cracks under mode I loading is achieved in a purpose build test set-up. Here, considering a 4 mm plate of normal strength / high strain hardening steel which has been found to display successive flipping of the slant crack face. While undergoing a shear band switch, such that the flipping mechanism is active, the plate tearing test is interrupted and the crack tip extracted for further investigation. The conducted X-ray tomography scans reveal the failure process ahead of the advancing crack tip to resemble the ductile slant crack growth governed by local thinning and moderate crack tip tunneling. However, small shear lips form at the outer free plate surface, well behind the 45-degree slant (tunneling) crack tip, as the flipping action engages. Upon further loading, the shear lips subsequently grow to form a set of secondary crack fronts at an angle to the primary tunneling slant crack. Eventually, these secondary crack fronts catch up on the primary slant crack front and overtake the growth to complete the shear band switch. Once the crack slants, an out-of-plane action occurs due to the loss of symmetry in the system. It is this out-of-plane action which is believed to set-off the flipping mechanism.
Creating model systems for catalysis with mass-selected nanoparticles: Characterization and properties

This PhD thesis reports research on the fundamental properties of nanoscale catalysts related to energy conversion processes. These processes and the connected materials will hopefully become more and more important in our future as humanity is shifting to renewable energy sources, but already today plenty of industrial heterogeneous catalysts are based on nanoparticles and their properties. The chapters in this thesis contain research on different processes and give examples of the possibilities of nanoscale catalyst materials. Because of the wide range of processes and materials involved, a brief summary of the included projects is given individually. If we were to switch to renewable energy sources, utilizing sunlight would be an obvious choice. With the use of a suitable photoabsorber and catalysts, sunlight can be directly used to drive the water splitting process generating O₂ in the oxygen evolution reaction (OER) and H₂ in the...
A resonant inelastic x-ray scattering study of overdamped spin excitations in slightly underdoped La$_{2-x}$Sr$_x$CuO$_4$ (LSCO) with $x = 0.12$ and 0.145 is presented. Three high-symmetry directions have been investigated: (1) the antinodal $(0,0)$ -> $(\frac{1}{2}, \frac{1}{2})$, (2) the nodal $(0,0)$ -> $(\frac{1}{2}, \frac{3}{2})$, and (3) the zone-boundary direction $(\frac{1}{2}, 0)$ -> $(\frac{1}{4}, \frac{1}{4})$ connecting these two. The overdamped excitations exhibit strong dispersions along (1) and (3), whereas a much more modest dispersion is found along (2). This is in strong contrast to the undoped compound La$_2$CuO$_4$ (LCO) for which the strongest dispersions are found along (1) and (2). The $t$ - $t'$ - $t''$ - $U$ Hubbard model used to explain the excitation spectrum of LCO predicts-for constant $U/t$-that the dispersion along (3) scales with $(t'/t)^2$. However, the diagonal hopping $t'$ extracted on LSCO using single-band models is low $(t'/t \sim -0.16)$ and decreasing with doping. We therefore invoked a two-orbital ($d_{x^2-y^2}$ and $d_{z^2}$) model which implies that $t'$ is enhanced. This effect acts to enhance the zone-boundary dispersion within the Hubbard model. We thus conclude that hybridization of $d_{x^2-y^2}$ states has a significant impact on the zone-boundary dispersion along (3). However, the diagonal hopping $t'$ extracted on LSCO using single-band models is low $(t'/t \sim -0.16)$ and decreasing with doping. We therefore invoked a two-orbital ($d_{x^2-y^2}$ and $d_{z^2}$) model which implies that $t'$ is enhanced. This effect acts to enhance the zone-boundary dispersion within the Hubbard model. We thus conclude that hybridization of $d_{x^2-y^2}$ and $d_{z^2}$ states has a significant impact on the zone-boundary dispersion within the Hubbard model.
dispersion in LSCO.

**General information**
- **State:** Published
- **Organisations:** Department of Physics, Neutrons and X-rays for Materials Physics, Universität Zürich, Ecole Polytechnique Federale de Lausanne (EPFL), Paul Scherrer Institut, University of Central Lancashire, Hokkaido University
- **Number of pages:** 8
- **Publication date:** 2017
- **Main Research Area:** Technical/natural sciences

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- **Volume:** 95
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- **Article number:** 214508
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  - BFI (2018): BFI-level 1
  - Web of Science (2018): Indexed yes
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  - 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
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  - 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
Dark excitations in monolayer transition metal dichalcogenides

Monolayers of transition metal dichalcogenides (TMDCs) possess unique optoelectronic properties, including strongly bound excitons and trions. To date, most studies have focused on optically active excitations, but recent experiments have highlighted the existence of dark states, which are equally important in many respects. Here, we use ab initio many-body calculations to unravel the nature of the dark excitations in monolayer MoSe₂, MoS₂, WSe₂, and WS₂. Our results show that all these monolayer TMDCs host dark states as their lowest neutral and charged excitations. We further show that dark excitons possess larger binding energies than their bright counterparts while the opposite holds for trions.

General information
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Organisations: Department of Physics, Theoretical Atomic-scale Physics, Center for Nanostructured Graphene
Authors: Deilmann, T. (Intern), Thygesen, K. S. (Intern)
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Journal: Physical Review B
Volume: 96
Issue number: 20
Article number: 201113
ISSN (Print): 2469-9950
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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
Deactivating Carbon Formation on a Ni/Al2O3 Catalyst under Methanation Conditions

The carbon formation causing deactivation during CO methanation was studied for a Ni/Al2O3 catalyst. Sulfur-free methanation at low temperature (573 K) for various lengths of time was followed by temperature-programmed hydrogenation (TPH) providing information on carbon types involved in the deactivation of the catalyst. Three main carbon hydrogenation peaks were evident from TPHs following methanation: ~460, ~650, and ~775 K. It is suggested that the ~460 K TPH peak was composed of two peaks: a surface carbide peak at 445–460 K, and a peak due to carbon dissolved into the nickel at 485 K based on CO and CH4 adsorption measurements and XRD analysis. The 650 and 775 K temperature peaks are assigned to polymerized carbon structures and the ~775 K peak was found to be the primary cause of deactivation as judged by a linear correlation between its amount and the degree of catalyst deactivation. The longer the duration of the methanation test, the more carbon was built up on the Ni surfaces and the highest observed amount was quantified to be as much as eight carbon atoms per Ni surface atom (8 C/Nsurf), which would roughly correspond to an average coverage of four monolayers of graphene. From H2 desorption measurements after reaction the 650 K TPH peak carbon structure is proposed to be partially hydrogenated, possibly resembling polycyclic aromatic-like carbon. The 775 K peak carbon species are likely more graphene-like. Results indicate that although carbon deposition nucleation may be initiated at the most active methanation sites, i.e., the Ni step sites, subsequent growth takes place over Ni terracesites. A strongly inhomogeneous carbon growth distribution over the Ni nanoparticle surfaces could also account for our findings. Similar to suggestions regarding catalyst deactivation in Fischer–Tropsch synthesis, a surface CH* coupling mechanism is likely taking place, and our results suggest these polymeric hydrocarbon species become more ordered, aromatic, and eventually graphene-like over time.

General information

State: Published
Organisations: Experimental Surface and Nanomaterials Physics, Department of Physics, Center for Electron Nanoscopy, Haldor Topsoe AS
Authors: Olesen, S. E. (Intern), Andersson, K. J. (Ekstern), Damsgaard, C. D. (Intern), Chorkendorff, I. (Intern)
Number of pages: 9
Defect Chemistry and Electrical Conductivity of Sm-Doped La_{1-x}Sr_{x}CoO_{3-δ} for Solid Oxide Fuel Cells

We have calculated the electrical conductivity of the solid oxide fuel cell (SOFC) cathode contact material La_{1-x}Sr_{x}CoO_{3-δ} at 900 K. Experimental trends in conductivity against x, and against δ for fixed x, are correctly reproduced for x ≤ 0.8. Furthermore, we have studied the chemistry of neutral and charged intrinsic and extrinsic defects (dopants) in La_{0.5}Sr_{0.5}CoO_{3} and have calculated the conductivity of the doped systems. In particular, we find that doping with Sm on the La site should enhance the conductivity, a prediction that is subsequently confirmed by electrical conductivity measurements.

General information

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Organisations: Department of Physics, Theoretical Atomic-scale Physics, Aisin Seiki, IMRA Europe
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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
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BFI (2013): BFI-level 1
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ISI indexed (2013): ISI indexed yes
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BFI (2012): BFI-level 1
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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
Detector response artefacts in spectral reconstruction

Energy resolved detectors are gaining traction as a tool to achieve better material contrast. K-edge imaging and tomography is an example of a method with high potential that has evolved on the capabilities of photon counting energy dispersive detectors. Border security is also beginning to see instruments taking advantage of energy resolved detectors. The progress of the field is halted by the limitations of the detectors. The limitations include nonlinear response for both x-ray intensity and x-ray spectrum. In this work we investigate how the physical interactions in the energy dispersive detectors affect the quality of the reconstruction and how corrections restore the quality. We have modeled detector responses for the primary detrimental effects occurring in the detector; escape peaks, charge sharing/loss and pileup. The effect of the change in the measured spectra is evaluated based on the artefacts occurring in the reconstructed images. We also evaluate the effect of a correction algorithm for reducing these artefacts on experimental data acquired with a setup using Multix ME-100 V-2 line detector modules. The artefacts were seen to introduce 20% deviation in the reconstructed attenuation coefficient for the uncorrected detector. We performed tomography experiments on samples with various materials interesting for security applications and found the SSIM to increase >; 5% below 60keV. Our work shows that effective corrections schemes are necessary for the accurate material classification in security application promised by the advent of high flux detectors for spectral tomography.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, University of Copenhagen
Authors: Olsen, U. L. (Intern), Christensen, E. D. (Ekstern), Khalil, M. (Intern), Gu, Y. (Intern), Kehres, J. (Intern)
Number of pages: 10
Publication date: 2017
Determination of low-strain interfaces via geometric matching

We present a general method for combining two crystals into an interface. The method finds all possible interfaces between the crystals with small coincidence cells and identifies the strain and area of the corresponding two-dimensional cells of the two crystal surfaces. We apply the method to the two semiconductor alloys InAs$_{1-x}$Sb$_x$ and Ga$_x$In$_{1-x}$As combined with a selection of pure metals or with NbTiN to create semiconductor/superconductor interfaces. The lattice constant of the alloy can be tuned by composition and we can extract the alloy lattice parameters corresponding to zero strain in both the metal and the alloy. The results can be used to suggest new epitaxially matched interfaces between two materials.

General information

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Organisations: Department of Physics, Theoretical Atomic-scale Physics, Neutrons and X-rays for Materials Physics, QuantumWise A/S
Authors: Jelver, L. (Intern), Larsen, P. M. (Intern), Stradi, D. (Ekstern), Stokbro, K. (Ekstern), Jacobsen, K. W. (Intern)
Number of pages: 7
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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
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Scopus rating (2014): SJR 2.762 SNIP 1.316 CiteScore 3.3
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Scopus rating (2011): SJR 3.326 SNIP 1.423 CiteScore 3.61
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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
Determining material parameters using phase-field simulations and experiments

A method to determine material parameters by comparing the evolution of experimentally determined 3D microstructures to simulated 3D microstructures is proposed. The temporal evolution of a dendritic solid-liquid mixture is acquired in situ using x-ray tomography. Using a time step from these data as an initial condition in a phase-field simulation, the computed structure is compared to that measured experimentally at a later time. An optimization technique is used to find the material parameters that yield the best match of the simulated microstructure to the measured microstructure in a global manner. The proposed method is used to determine the liquid diffusion coefficient in an isothermal Al-Cu alloy. However, the method developed is broadly applicable to other experiments in which the evolution of the three-dimensional microstructure is determined in situ. We also discuss methods to describe the local variation of the best-fit parameters and the fidelity of the fitting. We find a liquid diffusion coefficient that is different from that measured using directional solidification.

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Scopus rating (2016): CiteScore 5.67 SJR 3.21 SNIP 2.702
Web of Science (2016): Indexed yes
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<td>Scopus rating (2000): SJR 3.22 SNIP 2.164</td>
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<td>Scopus rating (1999): SJR 3.069 SNIP 2.167</td>
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Original language: English
Phase-field method, X-ray tomography, Coarsening, Al alloys, Temporal evolution

Electronic versions:
filestore.pdf
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Publication: Research - peer-review › Journal article – Annual report year: 2017

**Development and application of advanced methods for electronic structure calculations**
This thesis relates to improvements and applications of beyond-DFT methods for electronic structure calculations that are applied in computational material science. The improvements are of both technical and principal character.
The well-known GW approximation is optimized for accurate calculations of electronic excitations in two-dimensional materials by exploiting exact limits of the screened Coulomb potential. This approach reduces the computational time by an order of magnitude, enabling large scale applications. The GW method is further improved by including so-called vertex corrections. This turns out to yield ionization potentials and electron affinities that are in better agreement with experiments for both bulk and 2D materials. This newly developed method requires the calculation of an exchange-correlation kernel known from time-dependent DFT. The computational cost of the kernel is negligible compared with the cost of the GW calculation itself, and the kernel even improves the convergence performance. Literature shows and this thesis confirms that the representation of the individual atomic elements through their PAW setup crucially affects the results of GW calculations. For this reason, part of this thesis relates to developing and applying a new method for constructing so-called norm-conserving PAW setups, that are applicable to GW calculations by using a genetic algorithm. The effect of applying the new setups significantly affects the absolute band positions, both for bulk and 2D materials. The new PAW setups are used for producing most of the results presented in this thesis.

A lack of accurate experimental and theoretical data on adsorption energies, relevant to surface chemistry and catalysis, are identified. The RPA method and beyond, that is known to yield accurate ground state energies, is used to calculate accurate adsorption energies for a wide range of reactions. The results are in good agreement with experimental values, where available. Additionally, a database consisting of 200 highly accurate adsorption energies is constructed to benchmark the accuracy of current DFT functionals and to guide future development of new xc functionals for DFT, especially useful for surface science.

Given the accuracy of existing DFT functionals, they were in turn applied in search for catalysts to be used in electrochemical methanol production from methane. Two different types of surfaces were investigated for this reaction; the (110) surface of rutile transition metal oxides and a fairly new class of two-dimensional materials called MXenes. Promising candidates were found within the MXenes.

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**Relations**

Projects:
Development and application of advanced methods for electronic structure calculations
Publication: Research › Ph.D. thesis – Annual report year: 2017

**Development of measurement protocols for quantum magnetometry**

The work presented in this thesis revolves around quantum enhanced magnetic field sensing. The core of the study is the nitrogen-vacancy (NV) center, a point defect in the diamond lattice with atomic like properties and magnetic field susceptibility. The central task was to develop control schemes and protocols to enhance the lifetime and the coherences of the NV center with the overall goal of enhancing the capabilities of this sensor in the field of magnetometry. In order to realize complex protocols, a sophisticated software control of the measurement setup is required. A general software framework, termed Qudi, was designed and developed from scratch to improve drastically the measurement abilities and to facilitate the transfer of knowledge between the measurement protocols and the underlying physical idea. The transparent character of the core code, fully open to the scientific community, is serving as rigorous framework to benchmark the accuracy of current DFT functionals and to guide future development of new xc functionals for DFT, especially useful for surface science.

The measurement of magnetic fields in the high-frequency GHz regimes is challenging. In this thesis, a continuous dynamical decoupling protocol is developed and implemented, which extends the capabilities of the NV sensor to probe GHz signals with a narrow bandwidth. Moreover, the protocol protects the system from noise, attributed to the drive, and from external magnetic noise thereby prolonging the coherence time and reaching the lifetime limitation of the quantum states. We measured a coherence time of 1.43 ms at room temperature in a diamond crystal with a natural abundance of $^{13}$C atoms, resulting in a smallest detectable magnetic field strength of 4 nT at 1.6 GHz. Creating a protected qubit from a three-level system requires multiple drive fields addressing different transition frequencies. Continuous dynamical decoupling can protect the system from external magnetic noise, but typically introduces large drive noise to the system. The combination of on-resonant and off-resonant driving fields serves an approach to circumvent the challenges associated with drive noise. While on-resonant drive maintains a large energy gap in order to protect the sensor from external magnetic noise, the off-resonant drive creates AC-Stark shifted energy levels, thereby significantly reducing the
amount of drive noise on the three-level system. We experimentally demonstrate an improvement in coherence time, which is only limited by the second order contributions of the magnetic field noise while suppressing entirely the drive noise contributions. Further improvement can be achieved by a mere increase of the drive field as its noise is efficiently decoupled from the sensor.

Direct bonding of ALD Al₂O₃ to silicon nitride thin films

Direct bonding is an advanced joining technique for bonding of silicon based surfaces at low temperature without any specific surface pretreatment. The main purpose of this work is to develop new techniques to enhance the fabrication process for nanofluidic systems for in situ transmission electron microscopy (TEM) by improving low temperature annealing bonding strength when using atomic layer deposition of aluminum oxide. We have investigated and characterized bonding of Al₂O₃-Si₃N₄ (low-stress silicon rich nitride) and Al₂O₃-Si₂N₄ (stoichiometric nitride) thin films annealed from room temperature up to 600 degrees C without pretreatment prior to the pre bonding. We find that bonding of Al₂O₃-Si₃N₄ and Al₂O₃-Si₂N₄ is favorable in a temperature range from room temperature to 600 °C. We report bonding strength of 1300±150 mJ/m² comparable to and in some case even higher than that of other materials Al₂O₃ can be bonded to. Preliminary tests demonstrating a well-defined nanochannel system with~100 nm high channels successfully bonded and tests against leaks using optical fluorescence technique and transmission electron microscopy (TEM) characterization of liquid samples are also reported. Moreover, the current bonding method can be also used for further MEMS applications.
Diversity of trion states and substrate effects in the optical properties of an MoS$_2$ monolayer

Almost all experiments and future applications of transition metal dichalcogenide monolayers rely on a substrate for mechanical stability, which can significantly modify the optical spectra of the monolayer. Doping from the substrate might lead to the domination of the spectra by trions. Here we show by ab initio many-body theory that the negative trion (A$^-$) splits into three excitations, with both inter-and intra-valley character, while the positive counterpart (A$^+$) consists of only
one inter-valley excitation. Furthermore, the substrate enhances the screening, which renormalizes both band gap and exciton as well as the trion-binding energies. We verify that these two effects do not perfectly cancel each other, but lead to redshifts of the excitation energies for three different substrates ranging from a wide-bandgap semiconductor up to a metal. Our results explain recently found experimental splittings of the lowest trion line as well as excitation red-shifts on substrates.

General information
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Organisations: Department of Physics, Theoretical Atomic-scale Physics, Westfälische Wilhelms-Universität Münster
Authors: Drueppel, M. (Ekstern), Deilmann, T. (Intern), Krueger, P. (Ekstern), Rohlfing, M. (Ekstern)
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Main Research Area: Technical/natural sciences

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BFI (2013): BFI-level 1
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ISI indexed (2013): ISI indexed yes
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Scopus rating (2012): SJR 5.866 SNIP 2.829 CiteScore 8.32
ISI indexed (2012): ISI indexed yes
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ISI indexed (2011): ISI indexed no
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Source: FindIt
Dynamic breaking of a single gold bond

While one might assume that the force to break a chemical bond gives a measure of the bond strength, this intuition is misleading. If the force is loaded slowly, thermal fluctuations may break the bond before it is maximally stretched, and the breaking force will be less than the bond can sustain. Conversely, if the force is loaded rapidly it is more likely that the maximum breaking force is measured. Paradoxically, no clear differences in breaking force were observed in experiments on gold nanowires, despite being conducted under very different conditions. Here we explore the breaking behaviour of a single Au-Au bond and show that the breaking force is dependent on the loading rate. We probe the temperature and structural dependencies of breaking and suggest that the paradox can be explained by fast breaking of atomic wires and slow breaking of point contacts giving very similar breaking forces.

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ISI indexed (2011): ISI indexed no
Web of Science (2010): Indexed yes
Original language: English
Electronic versions:
ncomms15931.pdf
DOIs:
10.1038/ncomms15931
Source: FindIt
Source-ID: 2372367346
Effective modelling of acoustofluidic devices

In this thesis work we develop three models for involved systems in the field of microscale acoustofluidics. Because of the complexity of the systems studied, the aim of the Ph.d. project has been to make simplified and effective descriptions of these systems, capturing the most essential behaviour of the system, as opposed to making detailed calculations of idealised cases.

The effective models developed in this thesis concerns: 1) hydrodynamic particle-particle interactions in dense microparticle suspensions, 2) the acoustic field in mm-sized liquid-filled glass capillaries used for acoustic trapping, and 3) acoustic streaming patterns in the devices considered in model 2).

1) We derive an effective model for numerical studies of hydrodynamic particle-particle interactions in microfluidic high-concentration suspensions. A suspension of microparticles placed in a microfluidic channel and influenced by an external force, is described by a continuous particle-concentration field coupled to the continuity and Navier–Stokes equation for the solution. The hydrodynamic interactions are accounted for through the concentration dependence of the suspension viscosity, of the single-particle mobility, and of the momentum transfer between the particles and the suspension.

2) We derive a full 3D numerical model for the coupled acoustic fields in mm-sized water-filled glass capillaries, calculating pressure field in the liquid coupled to the displacement field of the glass channel, taking into account mixed standing and travelling waves as well as absorption. We model the connective tubing at the outlets, either as being free reflecting surfaces or perfect absorbers of outgoing acoustic waves, and we make an effective description of the mechanical actuation of the attached piezoelectric transducer.

3) Using the model for the acoustic field in glass capillary devices derived in 2), we make an effective model for calculating the acoustic streaming velocity in 3D. To do this, we use recent analytical results that allows calculation of the acoustic streaming field resulting from channel-wall oscillations in any direction, with significantly lower computational power requirements compared to previous methods, enabling full 3D calculations.
Effect of edge plasmons on the optical properties of MoS2 monolayer flakes

Finite MoS2 nanoparticles are known to support metallic edge states that are responsible for their catalytic activity. In this work we employ time-dependent density-functional theory (TDDFT) to study the influence of such edge states on the optical properties of triangular MoS2 monolayer flakes. We find that the edge states support collective plasmon-like excitations that couple strongly to the optical field leading to pronounced absorption peaks below the onset of interband transitions on the basal plane. Additionally, structural relaxation of the flakes can significantly distort the edge states. Thus, we observe that while an evenly-spaced edge configuration supports one-dimensional (1D) plasmon modes similar to those of an ideal 1D electron gas, the relaxed structures show mixed plasmon and single-electron excitations in the low-energy response. Our findings illustrate the sensitivity of the optical response of MoS2 nanostructures to the details of the edge configuration.

General information
State: Published
Organisations: Department of Physics, Theoretical Atomic-scale Physics, Center for Nanostructured Graphene, Aalto University
Authors: Rossi, T. P. (Ekstern), Winther, K. T. (Intern), Jacobsen, K. W. (Intern), Nieminen, R. M. (Ekstern), Puska, M. J. (Ekstern), Thygesen, K. S. (Intern)
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Scopus rating (2012): SJR 3.173 SNIP 1.378 CiteScore 3.57
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Web of Science (2012): Indexed yes
Scopus rating (2011): SJR 3.326 SNIP 1.423 CiteScore 3.61
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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
Substrate effects, Oxygen evolution reaction, Nickel oxyhydroxide, Nickel cerium, Nickel iron, Loading dependence, Conductivity, Electrochemical impedance spectroscopy
Electrochemical Insights into Platinum Catalysts for Fuel Cells

Development of sustainable energy production, conversion and storage technologies must be considered one of the major challenges of the 21st century. Insight and understanding of the oxygen reduction reaction is imperative in these pursuits. In this work electrochemical investigations and physical characterization of various model systems ranging from extended surfaces, to thin films and nanoparticle electrocatalysts have been presented and discussed. This has been done with a special focus on governing factors controlling the electroreduction of oxygen.

Preparation of Cu/Pt(111) near-surface alloys was conducted and compared to earlier results from our group. In lieu of the Cu amount in the 2nd atom layer the OH adsorption energy could be tuned. This was done for a range of Cu/Pt(111) samples which were investigated in alkaline media, revealing a Sabatier volcano relationship to the relative shift in OH adsorption potential. This work demonstrates, for the first time, that the OH binding energy indeed is a descriptor in alkaline as well as in acidic media. The apparent synergistic effects between the alkali cations and the electrodesurface of the Cu/Pt(111) combined with the optimization of the OH binding energy, resulted in extremely high specific oxygen reduction activities. The maximum ORR activity was recorded to be 100.7 ± 7.5 mA/cm² at 0.9 V vs. the reversible hydrogen electrode.

The Cu/Pt(111) system was also used to investigate the oxygen reduction reaction in the presence of poisoning anions from the electrolyte. These experiments revealed that catalyst with optimum activity in non-adsorbate-adsorbate interacting electrolytes, such as HClO₄, also resulted in catalytic surfaces with superior tolerances for phosphate. Suggesting scaling between OH and phosphate adsorption energies.

Results on Gd/Pt(111) samples revealed that compressive strain from Pt overlayer formation is of major importance for the observed oxygen reduction activity enhancement. In-situ GI-XRD studies revealed that the overlayer forms almost instantaneous once the electrode is immersed into the acidic electrolyte. Furthermore, the overlayer appeared to be very stable after accelerated stability test.

Pt and Pt-Gd thin film investigation was also conducted. Here X-ray characterization played a central role in ascertaining that oxygen incorporation into the alloy, due to the oxyphilic nature of Gd, was kept at a minimum. Stable Pt and Pt₅Gd thin films were produced and electrochemical characterization experiments revealed specific activities of 0.9 V vs. RHE of 9.0 ± 0.6 mA/cm² and stability retention of 83%. Both of these metrics were comparable to those reported for bulk polycrystalline Pt₅Gd samples in HClO₄ electrolyte.

A preliminary electrochemical study of in-house synthesized Pt-Y nanoparticles have also been presented revealing specific mass actives of 0.3 ± 0.1 A/mgPt in HClO₄. The study revealed that extensive optimizations of the Pt-Y nanoparticles are required and their performance is severely impeded by poor electrochemically active areas and maybe also non-conformity of their crystal phase structure.
Electromechanical Response of Polycrystalline Barium Titanate Resolved at the Grain Scale

Ferroic materials are critical components in many modern devices. Polycrystalline states of these materials dominate the market due to their cost effectiveness and ease of production. Studying the coupling of ferroic properties across grain boundaries and within clusters of grains is therefore critical for understanding bulk polycrystalline ferroic behavior. Here, three-dimensional X-ray diffraction is used to reconstruct a 3D grain map (grain orientations and neighborhoods) of a polycrystalline barium titanate sample and track the grain-scale non-180° ferroelectric domain switching strains of 139 individual grains in situ under an applied electric field. The map shows that each grain is located in a very unique local environment in terms of intergranular misorientations, leading to local strain heterogeneity in the as-processed state of the sample. While primarily dependent on the crystallographic orientation relative to the field directions, the response of individual grains is also heterogeneous. These unique experimental results are of critical importance both when building the starting conditions and considering the validity of grain-scale modeling efforts, and provide additional considerations in the design of novel ferroic materials.
Electronic excitations in two-dimensional materials and van der Waals heterostructures

General information
State: Published
Organisations: Department of Physics, Theoretical Atomic-scale Physics, Center for Nanostructured Graphene
Authors: Thygesen, K. S. (Intern)
Number of pages: 67
Publication date: 2017
Enabling Ultra Deep Hydrodesulfurization by Nanoscale Engineering of New Catalysts

The HYDECAT project was initiated to make a targeted effort in the field of hydrodesulfurization (HDS), which is the process where sulfur is removed from crude oil by addition of hydrogen to form hydrocarbons and hydrogen sulfide. This PhD thesis represents my share in the project.

Due to the adverse environmental and societal effects of sulfur emissions from on-road transportation, legislation has been continuously tightened, pushing oil refiners to produce ultra-low sulfur diesel (ULSD), with a maximum sulfur content of 15 ppm. Since these specifications are expected to be further tightened, the existing HDS catalysts fall short. Experiments were performed on a setup dedicated to testing minute amounts of well-defined catalytic systems in the ambient pressure gas phase HDS of the model compounds dibenzothiophene (DBT) and 4,6-dimethyldibenzothiophene (4,6-DMDBT). An existing µ-reactor platform connected to a high resolution time-of-flight mass spectrometer (TOF-MS) was modified and optimized for this specific reaction. The µ-reactor has a reaction volume of only 240 nL and can be operated between 0.1-5 bar and temperatures up to 400 °C. Only 0.01 % of the mixed gas flows from the two inlets, O1 and O2, is bypassed through the reaction chamber and exposed to the catalyst. A channel terminated by a narrow capillary ensures that the entire reaction gas volume can be directed into the TOF-MS by probing only 5·10¹⁴ molecules/s.

The low vapor pressure of both DBT and 4,6-DMDBT complicated the process of introducing them in their gaseous form into the µ-reactor at ambient pressure, and a specially designed flange with an incorporated ion source and internal heat tracing was implemented.

HDS of DBT and 4,6-DMDBT at 800 mbar on six mass-selected Pt samples were conducted. Two Pt samples of ~3 nm (185 kamu) and two samples of ~6 nm (1500 kamu) all showed that only the direct desulfurization (DDS) pathway was followed, hence resulting in biphenyl (BiPhe) and 3,3'-dimethylbiphenyl (3,3'-DMBiPhe), respectively. The same was observed for two samples of Pt single atoms. One 1500 kamu sample reached full conversion and was used to derive a sensitivity factor, x, relating the DBT and BiPhe signals, since most ionization cross sections were unknown. This was applied in all the following data interpretation. Large deviations between the, in theory, identical samples made it difficult to see any clear trends, and it was estimated that a reaction temperature difference of 30 °C could have induced the different activities observed.

Four NiMo-based samples were tested in the HDS of DBT. Two metallic NiMo samples of ~3.5 nm (134 kamu), and two in-flight sulfided NiMoSₓ samples - one of ~5 nm (200 kamu) and one of ~6.5 nm (440 kamu). X-ray photoelectron spectroscopy (XPS) and activity measurements emphasized the need for a sulfidation step prior to the reaction, since exposure to air revealed the formation of an oxide layer. Scanning transmission electron microscopy (STEM) images of the in-flight sulfided NiMoSₓ samples showed flat lying platelet-like particles in the 200 kamu sample and upright standing particles in the 440 kamu sample. When normalized to the amount of metal in each sample, the activity of the flat lying particles were exceeded by the activity of the upright standing particles by an order of magnitude, indicating that more active edge sites are exposed in the latter and thereby enabling better HDS activity.

General information
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Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics
Authors: Christoffersen, A. N. (Intern), Chorkendorff, I. (Intern)
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Enabling Ultra Deep Hydrodesulfurization by Nanoscale Engineering of New Catalysts
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Engineering design and analysis of an ITER-like first mirror test assembly on JET
The ITER first mirrors are the components of optical diagnostic systems closest to the plasma. Deposition may build up on the surfaces of the mirror affecting their ability to fulfil their function. However, physics modelling of this layer growth is fraught with uncertainty. A new experiment is underway on JET, under contract to ITER, with primary objective to test if,
under realistic plasma and wall material conditions and with ITER-like first mirror aperture geometry, deposits do grow on first mirrors. This paper describes the engineering design and analysis of this mirror test assembly. The assembly was installed in the 2014-15 shutdown and will be removed in the 2016-17 shutdown.

**General information**

**State:** Published

**Organisations:** Department of Physics, Plasma Physics and Fusion Energy, Culham Science Centre, ITER, Royal Institute of Technology, Ecole Polytechnique

**Authors:** Vizvary, Z. (Ekstern), Bourdel, B. (Ekstern), Garcia-Carrasco, A. (Ekstern), Lam, N. N. (Ekstern), Leipold, F. (Intern), Pitts, R. (Ekstern), Reichle, R. (Ekstern), Riccardo, V. (Ekstern), Rubel, M. (Ekstern), De Temmerman, G. (Ekstern), Thompson, V. (Ekstern), Widdowson, A. (Ekstern)

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

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- Web of Science (2017): Indexed yes
- BFI (2016): BFI-level 1
- Scopus rating (2016): CiteScore 1.14 SJR 0.579 SNIP 1.054
- BFI (2015): BFI-level 1
- Scopus rating (2015): SJR 0.682 SNIP 1.493 CiteScore 1.41
- Web of Science (2015): Indexed yes
- BFI (2014): BFI-level 1
- Scopus rating (2014): SJR 0.704 SNIP 1.215 CiteScore 1.2
- Web of Science (2014): Indexed yes
- BFI (2013): BFI-level 1
- Scopus rating (2013): SJR 0.614 SNIP 1.421 CiteScore 1.35
- ISI indexed (2013): ISI indexed yes
- BFI (2012): BFI-level 1
- Scopus rating (2012): SJR 0.626 SNIP 1.106 CiteScore 0.99
- ISI indexed (2012): ISI indexed yes
- BFI (2011): BFI-level 1
- Scopus rating (2011): SJR 0.674 SNIP 1.771 CiteScore 1.4
- ISI indexed (2011): ISI indexed yes
- BFI (2010): BFI-level 1
- Scopus rating (2010): SJR 0.44 SNIP 1.121
- BFI (2009): BFI-level 1
- Scopus rating (2009): SJR 0.647 SNIP 1.282
- BFI (2008): BFI-level 1
- Scopus rating (2008): SJR 0.547 SNIP 0.965
- Scopus rating (2007): SJR 0.678 SNIP 1.263
- Web of Science (2007): Indexed yes
- Scopus rating (2006): SJR 0.382 SNIP 0.809
- Scopus rating (2005): SJR 0.491 SNIP 1.361
- Scopus rating (2004): SJR 0.97 SNIP 0.609
- Scopus rating (2003): SJR 0.554 SNIP 0.989
- Scopus rating (2002): SJR 1.158 SNIP 0.957
- Scopus rating (2001): SJR 0.406 SNIP 1.072
- Web of Science (2001): Indexed yes
Evaluation of HOPG mounting possibilities for multiplexing spectrometers

Four different methods for mounting HOPG analyzer crystals on Si holders have been evaluated in the design process of the new multiplexing spectrometer CAMEA. Contrary to neutron optics used in standard spectrometers, the new instrument concept employs a series of analyzer segments behind each other where the neutrons have to pass through the bonding compound of the different analyzer crystals. The different methods, namely screws, shellac, indium soldering and clips, have been evaluated with regards to background, transmission, cooling, activation and handling. The results presented here will give valuable input for future CAMEA-type spectrometers currently planned and designed at various neutron sources.

General information
State: Published
Organisations: Department of Physics, Ecole Polytechnique Federale de Lausanne (EPFL), Paul Scherrer Institut
Authors: Groitl, F. (Ekstern), Bartkowiak, M. (Ekstern), Bergmann, R. M. (Ekstern), Birk, J. O. (Intern), Marko, M. (Ekstern), Bolthaldner, A. (Ekstern), Graf, D. (Ekstern), Niedermayer, C. (Ekstern), Rueegg, C. (Ekstern), Rønnow, H. M. (Ekstern)
Number of pages: 6
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 1.333 SJR 0.814 CiteScore 1.48
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.44 SJR 0.866 SNIP 1.354
The impact of ion pressure dynamics on $E \times B$ mean flows is investigated. Using a simplified, two-dimensional, drift ordered fluid model in the thin-layer approximation, three stresses in addition to the Reynolds stress are shown to modify the $E \times B$ mean flow. These additional terms in the stress tensor all require ion pressure fluctuations. Quasi-linear analysis shows that these additional stresses are as important as the Reynolds stress and hence must be taken into account in...
analysis of transport barriers in which sheared E x B mean flows are key ingredients.

General information
State: Published
Organisations: Plasma Physics and Fusion Energy, Department of Physics
Authors: Madsen, J. (Intern), Rasmussen, J. J. (Intern), Naulin, V. (Intern), Nielsen, A. H. (Intern)
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BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.08 SJR 0.999 SNIP 1.052
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.874 SNIP 0.908 CiteScore 1.02
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.153 SNIP 1.195 CiteScore 1.69
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.114 SNIP 1.224 CiteScore 1.7
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.439 SNIP 1.255 CiteScore 1.83
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.221 SNIP 1.27 CiteScore 2.09
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.46 SNIP 1.283
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.592 SNIP 1.317
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.547 SNIP 1.363
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.483 SNIP 1.184
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.452 SNIP 1.454
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.4 SNIP 1.448
Fabrication of 3D electrodes for subretinal photovoltaic stimulation

General information
State: Published
Organisations: Department of Micro- and Nanotechnology, Silicon Microtechnology, Experimental Surface and Nanomaterials Physics, Aarhus University Hospital
Authors: Davidsen, R. S. (Intern), Keller, S. S. (Intern), Bek, T. (Ekstern), Hansen, O. (Intern)
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Event: Abstract from The Eye and the Chip 2017, Detroit, United States.
Main Research Area: Technical/natural sciences

Fast-ion transport in low density L-mode plasmas at TCV using FIDA spectroscopy and the TRANSP code

Experiments with the new neutral beam injection source of TCV have been performed with high fast-ion fractions (>20%) that exhibit a clear reduction of the loop voltage and a clear increase of the plasma pressure in on- and off-axis heating configurations. However, good quantitative agreement between the experimental data and TRANSP predictions is only found when including strong additional fast-ion losses. These losses could in part be caused by turbulence or MHD activity as, e.g., high frequency modes near the frequency of toroidicity induced Alfvén eigenmodes are observed. In addition, a newly installed fast-ion D-alpha (FIDA) spectroscopy system measures strong passive radiation and, hence, indicates the presence of high background neutral densities such that charge-exchange losses are substantial. Also the active radiation measured with the FIDA diagnostic, as well as data from a neutral particle analyzer, suggest strong fast-ion losses and large neutral densities. The large neutral densities can be justified since high electron temperatures (3–4 keV), combined with low electron densities (about 2 X 10¹⁹ m⁻³) yield long mean free paths of the neutrals which are penetrating from the walls.

General information
State: Published
Authors: Geiger, B. (Ekstern), Karpushov, A. (Ekstern), Duval, B. P. (Ekstern), Marini, C. (Ekstern), Sauter, O. (Ekstern), Andrébe, Y. (Ekstern), Testa, D. (Ekstern), Schneider, P. (Ekstern), Salewski, M. (Intern)
Number of pages: 15
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Main Research Area: Technical/natural sciences
FELIX: an algorithm for indexing multiple crystallites in X-ray free-electron laser snapshot diffraction images

A novel algorithm for indexing multiple crystals in snapshot X-ray diffraction images, especially suited for serial crystallography data, is presented. The algorithm, FELIX, utilizes a generalized parametrization of the Rodrigues-Frank space, in which all crystal systems can be represented without singularities. The new algorithm is shown to be capable of indexing more than ten crystals per image in simulations of cubic, tetragonal and monoclinic crystal diffraction patterns. It is also used to index an experimental serial crystallography dataset from lysozyme microcrystals. The increased number of indexed crystals is shown to result in a better signal-to-noise ratio, and fewer images are needed to achieve the same data quality as when indexing one crystal per image. The relative orientations between the multiple crystals indexed in an image show a slight tendency of the lysozme microcrystals to adhere on (110) facets.

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Department of Physics, Neutrons and X-rays for Materials Physics, Theoretical Atomic-scale Physics, Deutsches Elektronensynchroton DESY
Authors: Beyerlein, K. R. (Ekstern), White, T. A. (Ekstern), Yefanov, O. (Ekstern), Gati, C. (Ekstern), Kazantsev, I. G. (Intern), Gade-Nielsen, N. F. (Intern), Larsen, P. M. (Intern), Chapman, H. N. (Ekstern), Schmidt, S. (Intern)
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Web of Science (2017): Indexed Yes
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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
Ferroelectric domain continuity over grain boundaries

Formation and mobility of domain walls in ferroelectric materials is responsible for many of their electrical and mechanical properties. Domain wall continuity across grain boundaries has been observed since the 1950's and is speculated to affect the grain boundary-domain interactions, thereby impacting macroscopic ferroelectric properties in polycrystalline systems. However, detailed studies of such correlated domain structures across grain boundaries are limited. In this work, we have developed the mathematical requirements for domain wall plane matching at grain boundaries of any given orientation. We have also incorporated the effect of grain boundary ferroelectric polarization charge created when any two domains meet at the grain boundary plane. The probability of domain wall continuity for three specific grain misorientations is studied. Use of this knowledge to optimize processing techniques in manipulating the microstructure and domain structure to result in desired interactions between neighbouring grains could prove to be beneficial for future polycrystalline ferroelectric materials.

General information

State: Published
Organisations: Department of Physics, University of New South Wales, Ecole Polytechnique Federale de Lausanne (EPFL)
Authors: Mantri, S. (Ekstern), Oddershede, J. (Intern), Damjanovic, D. (Ekstern), Daniels, J. E. (Ekstern)
Pages: 400-405
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Main Research Area: Technical/natural sciences
Field-induced reentrant magnetoelectric phase in LiNiPO₄

Using pulsed magnetic fields up to 30 T we have measured the bulk magnetization and electrical polarization of LiNiPO₄ and have studied its magnetic structure by time-of-flight neutron Laue diffraction. Our data establish the existence of a reentrant magnetoelectric phase between 19 T and 21 T. We show that a magnetized version of the zero field commensurate structure explains the magnetoelectric response quantitatively. The stability of this structure suggests a field-dependent spin anisotropy. Above 21 T, amagnetoelectrically inactive, short-wavelength incommensurate structure is identified. Our results demonstrate the combination of pulsed fields with epithermal neutron Laue diffraction as a powerful method to probe even complex phase diagrams in strong magnetic fields.
Formation Mechanism of Maghemite Nanoflowers Synthesized by a Polyol-Mediated Process

Magnetic nanoparticles are being developed as structural and functional materials for use in diverse areas, including biomedical applications. Here, we report the synthesis of maghemite (γ-Fe₂O₃) nanoparticles with distinct morphologies: single-core and multicore, including hollow spheres and nanoflowers, prepared by the polyol process. We have used sodium acetate to control the nucleation and assembly process to obtain the different particle morphologies. Moreover, from samples obtained at different time steps during the synthesis, we have elucidated the formation mechanism of the nanoflowers: the initial phases of the reaction present a lepidocrocite (γ-FeOOH) structure, which suffers a fast dehydroxylation, transforming to an intermediate “undescribed” phase, possibly a partly dehydroxylated lepidocrocite, which after some incubation time evolves to maghemite nanoflowers. Once the nanoflowers have been formed, a crystallization process takes place, where the γ-Fe₂O₃ crystallites within the nanoflowers grow in size (from ~11 to 23 nm), but the particle size of the flower remains essentially unchanged (~60 nm). Samples with different morphologies were coated with citric acid and their heating capacity in an alternating magnetic field was evaluated. We observe that nanoflowers with large cores (23 nm, controlled by annealing) densely packed (tuned by low NaAc concentration) offer 5 times enhanced heating capacity compared to that of the nanoflowers with smaller core sizes (15 nm), 4 times enhanced heating effect compared to that of the hollow spheres, and 1.5 times enhanced heating effect compared to that of single-core nanoparticles (36 nm) used in this work.
From concept to in vivo testing: Microcontainers for oral drug delivery
This work explores the potential of polymeric micrometer sized devices (microcontainers) as oral drug delivery systems (DDS). Arrays of detachable microcontainers (D-MCs) were fabricated on a sacrificial layer to improve the handling and facilitate the collection of individual D-MCs. A model drug, ketoprofen, was loaded into the microcontainers using supercritical CO2 impregnation, followed by deposition of an enteric coating to protect the drug from the harsh gastric environment and to provide a fast release in the intestine. In vitro, in vivo and ex vivo studies were performed to assess the viability of the D-MCs as oral DDS. D-MCs improved the relative oral bioavailability by 180% within 4h, and increased the absorption rate by 2.4 times compared to the control. This work represents a significant step forward in the translation of these devices from laboratory to clinic.
Global numerical modeling of magnetized plasma in a linear device

Understanding the turbulent transport in the plasma-edge in fusion devices is of utmost importance in order to make precise predictions for future fusion devices. The plasma turbulence observed in linear devices shares many important features with the turbulence observed in the edge of fusion devices, and are easier to diagnose due to lower temperatures and a better access to the plasma. In order to gain greater insight into this complex turbulent behavior, numerical simulations of plasma in a linear device are performed in this thesis.

Here, a three-dimensional drift-fluid model is derived from first principles for a magnetized plasma in a linear device. To account for the fluctuations at the same level as the background plasma, the traditional split between background and fluctuations has not been made. The model is implemented using the BOUT++ framework and is solved numerically. Special attention is given to the treatment of the singularity at the cylinder axis, and at the inversion of the non-linear elliptic equation, which is done to obtain the electrical potential. The evolution of the plasma through the steady-state, linear phase, and turbulent phase is investigated and compared for different B-field strengths. It is found that drift-waves are responsible for the onset of turbulence, and that the turbulent radial flux is causing a flattening of the density profiles. Coherent structures from the intermittent radial flux in the turbulent state are investigated.

Results of simulations using the Boussinesq approximation is compared to full simulations. It is found that the Boussinesq approximation leads to an unphysical increase of the electrical potential as ions and electrons are lost at a different rate. Finally, the results from the full simulations are compared with simulations performed at different ionization levels, using a simple model for plasma interaction with neutrals. It is found that the steady state and the saturated state of the system bifurcates when the neutral interaction dominates the electron-ion collisions.
Glycine buffered synthesis of layered iron(II)-iron(III) hydroxides (green rusts)
Layered Fe(II)-Fe(III) hydroxides (green rusts, GRs) are efficient reducing agents against oxidizing contaminants such as chromate, nitrate, selenite, and chlorinated solvents. In this study, we adopted a buffered precipitation approach where glycine (GLY) was used in the synthesis of sulfate-interlayered GR (GRSO4) by aerial oxidation of Fe(II) or co-precipitation by adding Fe(III) salt to an aqueous solution of Fe(II) at constant pH. In both the oxidation and the co-precipitation methods pure crystalline GRSO4 was precipitated in the presence of 70mM GLY (pH 8.0), whereas in the absence of GLY, synthesis failed under similar conditions. Glycine functions as both a pH buffer and a ligand; Fe(II)-GLY complexes serve as a source of base (Fe(II)-GLY+H2O→Fe(II)+H-GLY+OH(-)) during GR formation, supplying about 45% of the total base required for the synthesis. The GLY buffer decreases pH fluctuations during base addition and hence allows for fast GRSO4 precipitation, minimizing byproduct formation. The use of other pH buffers [4-(2-hydroxyethyl)piperazine-1-ethanesulfonic acid and 2-amino-2-(hydroxymethyl)-1,3-propanediol] was also tested but failed. Mössbauer spectroscopy, X-ray diffraction, Fourier transform infrared, transmission electron microscopy, and Fe(II) measurements confirmed the purity, stoichiometry, and pyroaurite-type structure of the obtained GRSO4. The formula of GRSO4 was found to be Fe(II)4.08Fe(III)1.98(OH)11.6(SO4)1.00, and the tabular GR crystals had a lateral size of 100-500nm and a thickness of about 40nm. Upscaling of the synthesis by either 25 times in volume or 20 times in Fe(II) concentration resulted in pure GRSO4 products. Compared with the conventional unbuffered GRSO4 synthesis method, the present method can provide pure products with a controllable, fast, and low-cost process.
Grain interaction mechanisms leading to intragranular orientation spread in tensile deformed bulk grains of interstitial-free steel

The spatially resolved intragranular orientation spread in two representative bulk grains of interstitial-free steel deformed to 9% tension has been investigated. A three-dimensional X-ray diffraction microscopy experiment revealed that the two similarly oriented grains are both embedded in local environments representing the bulk texture, yet their deformation-
induced rotations are very different. The ALAMEL model is employed to analyse the grain interaction mechanisms. Predictions of this model qualitatively agree with the directionality and magnitude of the experimental orientation spread. However, quantitative agreement requires fine-tuning of the boundary conditions. The majority of the modelled slip is accounted for by four slip systems also predicted to be active by the classical Taylor model in uniaxial tension, and most of the orientation spread along the grain boundaries is caused by relative variations in the activities of these. Although limited to two grains, the findings prove that shear at the grain boundaries as accounted for by the ALAMEL model is a dominant grain interaction mechanism.
Graphite nodules in fatigue-tested cast iron characterized in 2D and 3D
Thick-walled ductile iron casts have been studied by applying (i) cooling rate calculations by FVM, (ii) microstructural characterization by 2D SEM and 3D X-ray tomography techniques and (iii) fatigue testing of samples drawn from components cast in sand molds and metal molds. An analysis has shown correlations between cooling rate, structure and fatigue strengths demonstrating the benefit of 3D structural characterization to identify possible causes of premature fatigue failure of ductile cast iron.
A multiscale density functional theory-quantum mechanics/molecular mechanics (DFT-QM/MM) scheme is presented, based on an efficient electrostatic coupling between the electronic density obtained from a grid-based projector augmented wave (GPAW) implementation of density functional theory and a classical potential energy function. The scheme is implemented in a general fashion and can be used with various choices for the descriptions of the QM or MM regions. Tests on H₂O clusters, ranging from dimer to decamer show that no systematic energy errors are introduced by the coupling that exceeds the differences in the QM and MM descriptions. Over 1 ns of liquid water, Born-Oppenheimer QM/MM molecular dynamics (MD) are sampled combining 10 parallel simulations, showing consistent liquid water structure over the QM/MM border. The method is applied in extensive parallel MD simulations of an aqueous solution of the diplatinum \( [\text{Pt}_2(\text{P}_2\text{O}_5\text{H}_2)^4]^- \) complex (PtPOP), spanning a total time period of roughly half a nanosecond. An average Pt-Pt distance deviating only 0.01 Å from experimental results, and a ground-state Pt-Pt oscillation frequency deviating by 

**General Information**

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Organisations: Department of Chemistry, Department of Physics, Theoretical Atomic-scale Physics, NanoChemistry, University of Iceland, Aalto University
Pages: 6010–6022
Highly Anisotropic in-Plane Excitons in Atomically Thin and Bulklike 1T'-ReSe₂

Atomically thin materials such as graphene or MoS₂ are of high in-plane symmetry. Crystals with reduced symmetry hold the promise for novel optoelectronic devices based on their anisotropy in current flow or light polarization. Here, we present polarization-resolved optical transmission and photoluminescence spectroscopy of excitons in 1T'-ReSe₂. On reducing the crystal thickness from bulk to a monolayer, we observe a strong blue shift of the optical band gap from 1.37 to 1.50 eV. The excitons are strongly polarized with dipole vectors along different crystal directions, which persist from bulk down to monolayer thickness. The experimental results are well reproduced by ab initio calculations based on the
GW-BSE approach within LDA+GdW approximation. The excitons have high binding energies of 860 meV for the monolayer and 120 meV for bulk. They are strongly confined within a single layer even for the bulk crystal. In addition, we find in our calculations a direct band gap in 1T'-ReSe₂ regardless of crystal thickness, indicating weak interlayer coupling effects on the band gap characteristics. Our results pave the way for polarization-sensitive applications, such as optical logic circuits operating in the infrared spectral region.
High Specific and Mass Activity for the Oxygen Reduction Reaction for Thin Film Catalysts of Sputtered Pt₃Y

Fuel cells have the potential to play an important role in sustainable energy systems, provided that catalysts with higher activity and stability are developed. In this work, it is found that thin alloy films of single-target cosputtered platinum-yttrium exhibit up to seven times higher specific activity (13.4 ± 0.4 mA cm⁻²) for the oxygen reduction reaction (ORR) than polycrystalline platinum, and up to one order of magnitude higher mass activity (3.5 ± 0.3 A mg⁻¹) than platinum nanoparticles. These alloys have the highest reported ORR activity for an as-deposited material, i.e., without any additional chemical or thermal treatment. The films show an improvement in stability over the same materials in nanoparticulate form. Physical characterization shows that the thin films form a platinum overlayer supported on an underlying alloy. The high activity is likely related to compressive strain in that overlayer. As sputtering can be used to mass-produce fuel cell electrodes, the results open new possibilities for the preparation of platinum-rare earth metal alloy catalysts in commercial devices.
Huge Trionic Effects in Graphene Nanoribbons

One- and two-dimensional materials are being intensively investigated due to their interesting properties for next-generation optoelectronic devices. Among these, armchair-edged graphene nanoribbons are very promising candidates with optical properties that are dominated by excitons. In the presence of additional charges, trions (i.e., charged excitons) can occur in the optical spectrum. With our recently developed first-principle many-body approach (Phys. Rev. Lett. 116, 196804), we predict strongly bound trions in free-standing nanoribbons with large binding energies of 140-660 meV for widths of 14.6-3.6 Å. Both for the trions and for the excitons, we observe an almost linear dependency of their binding energies on the band gap. We observe several trion states with different character derived from the corresponding excitons. Because of the large bindings energies, this opens a route to applications by which optical properties are easily manipulated, for example, by electrical fields.
Hydrodynamics of microbial filter feeding

Microbial filter feeders are an important group of grazers, significant to the microbial loop, aquatic food webs, and biogeochemical cycling. Our understanding of microbial filter feeding is poor, and, importantly, it is unknown what force microbial filter feeders must generate to process adequate amounts of water. Also, the trade-off in the filter spacing remains unexplored, despite its simple formulation: A filter too coarse will allow suitably sized prey to pass unintercepted, whereas a filter too fine will cause strong flow resistance. We quantify the feeding flow of the filter-feeding choanoflagellate Diaphanoeca grandis using particle tracking, and demonstrate that the current understanding of microbial filter feeding is inconsistent with computational fluid dynamics (CFD) and analytical estimates. Both approaches underestimate observed filtration rates by more than an order of magnitude; the beating flagellum is simply unable to draw enough water through the fine filter. We find similar discrepancies for other choanoflagellate species, highlighting an apparent paradox. Our observations motivate us to suggest a radically different filtration mechanism that requires a flagellar vane (sheet), something notoriously difficult to visualize but sporadically observed in the related choanoocytes (sponges). A CFD model with a flagellar vane correctly predicts the filtration rate of D. grandis, and using a simple model we can account for the filtration rates of other microbial filter feeders. We finally predict how optimum filter mesh size increases with cell size in microbial filter feeders, a prediction that accords very well with observations. We expect our results to be of significance for small-scale biophysics and trait-based ecological modeling.

Recent experiments on II–IV–V₂ type nitrides and phosphides have shown that these materials are potential candidates as photovoltaic absorbers. The materials space for such light absorbers can be expanded by elemental substitution of the different species, and thanks to the small energy difference of the polymorphs, the space can be extended by tuning the atomic structure as well. Using electronic structure calculations, we explore chalcopyrite, kesterite, and wurtzite polymorphs of II–IV–V₂ and III–III–V₂ materials for light absorption especially in the visible range. Based on the thermodynamic stability, band gap, and charge carrier effective masses, we discuss the possibility for the materials containing nontoxic elements to act as PV absorbers. Additionally, the systematic mapping of the materials space provides trends in thermodynamic and electronic properties which can be exploited further to tune these properties via elemental substitution and/or alloying.
Importance sampling of rare events in chaotic systems

Finding and sampling rare trajectories in dynamical systems is a difficult computational task underlying numerous problems and applications. In this paper we show how to construct Metropolis-Hastings Monte-Carlo methods that can efficiently sample rare trajectories in the (extremely rough) phase space of chaotic systems. As examples of our general framework we compute the distribution of finite-time Lyapunov exponents (in different chaotic maps) and the distribution of escape times (in transient-chaos problems). Our methods sample exponentially rare states in polynomial number of samples (in both low- and high-dimensional systems). An open-source software that implements our algorithms and reproduces our results can be found in reference [J. Leitao, A library to sample chaotic systems, 2017, https://github.com/jorgecarleitao/chaospp].

General information
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Organisations: Department of Physics, Max-Planck-Institute for the Physics of Complex Systems, University of Minho, University of Porto, University of Sydney
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Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
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BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.514 SNIP 0.654 CiteScore 1.13
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
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BFI (2013): BFI-level 1
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Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.861 SNIP 0.867 CiteScore 1.51
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.034 SNIP 0.916 CiteScore 1.6
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.101 SNIP 0.863
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.974 SNIP 0.81
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Scopus rating (2006): SJR 1.186 SNIP 0.964
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Scopus rating (2004): SJR 1.376 SNIP 0.986
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.484 SNIP 0.96
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Scopus rating (2002): SJR 1.527 SNIP 1.216
Scopus rating (2001): SJR 1.91 SNIP 1.164
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 0.783 SNIP 1.405
Web of Science (2000): Indexed yes
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Bibliographical note
Open Access This is an open access article distributed under the terms of the Creative Commons Attribution License (http://creativecommons.org/licenses/by/4.0), which permits unrestricted use, distribution, and reproduction in any
Improved orientation sampling for indexing diffraction patterns of polycrystalline materials

Orientation mapping is a widely used technique for revealing the microstructure of a polycrystalline sample. The crystalline orientation at each point in the sample is determined by analysis of the diffraction pattern, a process known as pattern indexing. A recent development in pattern indexing is the use of a brute-force approach, whereby diffraction patterns are simulated for a large number of crystalline orientations and compared against the experimentally observed diffraction pattern in order to determine the most likely orientation. Whilst this method can robustly identify orientations in the presence of noise, it has very high computational requirements. In this article, the computational burden is reduced by developing a method for nearly optimal sampling of orientations. By using the quaternion representation of orientations, it is shown that the optimal sampling problem is equivalent to that of optimally distributing points on a four-dimensional sphere. In doing so, the number of orientation samples needed to achieve a desired indexing accuracy is significantly reduced. Orientation sets at a range of sizes are generated in this way for all Laue groups and are made available online for easy use.

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Authors: Larsen, P. M. (Intern), Schmidt, S. (Intern)
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BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 1.346 SJR 1.635 CiteScore 2.72
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
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ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Improved positioning and detectability of microparticles in droplet microfluidics using two-dimensional acoustophoresis

We have fabricated a silicon-glass two-phase droplet microfluidic system capable of generating sub 100 μm-sized, ϕ = (74 ± 2) μm, spherical droplets at rates of up to hundreds of hertz. By implementing a two-dimensional (2D) acoustophoresis particle-positioning method, we show a fourfold improvement in both vertical and lateral particle positioning inside the droplets compared to unactuated operation. The efficiency of the system has been optimized by incorporating aluminum matching layers in the transducer design permitting biocompatible operational temperatures (<37 °C). Furthermore, by using acoustic actuation, (99.8 ± 0.4)% of all encapsulated microparticles can be detected compared to only (79.0 ± 5.1)% for unactuated operation. In our experiments we observed a strong ordering of the microparticles in distinct patterns within the droplet when using 2D acoustophoresis; to explain the origin of these patterns we simulated numerically the fluid flow inside the droplets and compared with the experimental findings.
Acoustophoresis, Droplet microfluids, Ultrasonic standing wave, Microparticle detection, Microparticle manipulation

Original language: English

Acoustophoresis, Droplet microfluids, Ultrasonic standing wave, Microparticle detection, Microparticle manipulation

DOIs:
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.

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Indoor measurement of angle resolved light absorption by antireflective glass in solar panels
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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
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Publisher: IEEE
Main Research Area: Technical/natural sciences
Induced Mesocrystal-Formation, Hydrothermal Growth and Magnetic Properties of α-Fe₂O₃ Nanoparticles in Salt-Rich Aqueous Solutions

Iron oxide nanoparticles are widely prevalent in our aqueous environment (e.g., streams, seawater, hydrothermal vents). Their aggregation and crystal growth depend on their chemical surroundings, for instance just a change in pH or salt concentration can greatly affect this. In turn this influences their properties, mobility, fate, and environmental impact. We studied the growth of α-Fe₂O₃ (hematite), starting from 8 nm hematite particles in weakly acidic (HNO₃) aqueous suspension with different states of particle aggregation, using salt (NaCl and NaH₂PO₄) to control their initial aggregation state. The samples were then subject to hydrothermal treatment at 100-140 degrees C. We followed the development in aggregation state and particle size by dynamic light scattering, X-ray diffraction, small angle neutron scattering and transmission electron microscopy, and the magnetic properties by Mossbauer spectroscopy. The addition of NaCl and NaH₂PO₄ both led to aggregation, but NaCl led to linear chains of hematite nanoparticles (oriented parallel to their hexagonal c-axis), such that the crystalline lattice planes of neighboring hematite particles were aligned. However, despite this oriented alignment, the particles did not merge and coalesce. Rather they remained stable as mesocrystals until heat-treated. In turn, the addition of NaCl significantly increases the rate of growth during hydrothermal treatment, probably because the nanoparticles, due to the chain formation, are already aligned and in close proximity. With hydrothermal treatment, the magnetic properties of the particles transform from those characteristic of small (aggregated) hematite nanoparticles to those of particles with more bulk-like properties such as Morin transition and suppression of superparamagnetic relaxation, in correspondence with the growth of particle size.

General information
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Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics, Neutrons and X-rays for Materials Physics, Center for Electron Nanoscopy
Authors: Brok, E. (Intern), Larsen, J. (Intern), Varón, M. (Intern), Hansen, T. W. (Intern), Frandsen, C. (Intern)
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Web of Science (2016): Indexed yes
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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
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Authors: Skyggebjerg, L. K. (Intern)
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Influence of polyvinylpyrrolidone on optical, electrical, and dielectric properties of poly(2-ethyl-2-oxazoline)-polyvinylpyrrolidone blends

General information
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Organisations: Department of Physics, Siddaganga Institute of Technology
Authors: Shubha, A. (Ekstern), Manohara, S. (Ekstern), Gerward, L. (Intern)
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In operando studies of an yttria stabilized zirconia electrolyte supported symmetric solid oxide cell by Dark field X-ray Microscopy at ID06

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

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Main Research Area: Technical/natural sciences
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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 °C 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
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In situ characterization of heterogeneous catalysts

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Organisations: Center for Electron Nanoscopy, Department of Physics, Experimental Surface and Nanomaterials Physics
Authors: Damsgaard, C. D. (Intern)
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Event: Abstract from Frontiers in Materials Processing Applications, Research and Technology, Bordeaux, France.
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In situ microscopy of formation of nickel-based bimetallic nanoparticles

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Organisations: Center for Electron Nanoscopy, Department of Physics, Experimental Surface and Nanomaterials Physics
Authors: Damsgaard, C. D. (Intern)
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Electronic versions: Untitled.pdf

In-Situ X-ray Tomography Study of Cement Exposed to CO₂ Saturated Brine
For successful CO₂ storage in underground reservoirs, the potential problem of CO₂ leakage needs to be addressed. A profoundly improved understanding of the behavior of fractured cement under realistic subsurface conditions including elevated temperature, high pressure and the presence of CO₂ saturated brine is required. Here, we report in situ X-ray micro computed tomography (µ-CT) studies visualizing the microstructural changes upon exposure of cured Portland cement with an artificially engineered leakage path (cavity) to CO₂ saturated brine at high pressure. Carbonation of the bulk cement, self-healing of the leakage path in the cement specimen, and leaching of CaCO₃ were thus directly observed. The precipitation of CaCO₃, which is of key importance as a possible healing mechanism of fractured cement, was found to be enhanced in confined regions having limited access to CO₂. For the first time, the growth kinetics of CaCO₃ under more realistic well conditions have thus been estimated quantitatively. Combining the µ-CT observations with scanning electron microscopy resulted in a detailed understanding of the processes involved in the carbonation of cement.

General information
State: Published
Interlayer Excitons and Band Alignment in MoS$_2$/hBN/WSe$_2$ van der Waals Heterostructures

van der Waals heterostructures (vdWH) are ideal systems for exploring light-matter interactions at the atomic scale. In particular, structures with a type-II band alignment can yield detailed insight into carrier-photon conversion processes, which are central to, for example, solar cells and light-emitting diodes. An important first step in describing such processes is to obtain the energies of the interlayer exciton states existing at the interface. Here we present a general first-principles method to compute the electronic quasi-particle (QP) band structure and excitonic binding energies of incommensurate vdWHs. The method combines our quantum electrostatic heterostructure (QEH) model for obtaining the dielectric function with the many-body GW approximation and a generalized 2D Mott-Wannier exciton model. We calculate the level alignment together with intra- and interlayer exciton binding energies of bilayer MoS$_2$/WSe$_2$ with and without intercalated hBN layers, finding excellent agreement with experimental photoluminescence spectra. A comparison to density functional theory calculations demonstrates the crucial role of self-energy and electron-hole interaction effects.
Interlayer excitons in a bulk van der Waals semiconductor

Bound electron-hole pairs called excitons govern the electronic and optical response of many organic and inorganic semiconductors. Excitons with spatially displaced wave functions of electrons and holes (interlayer excitons) are important for Bose-Einstein condensation, superfluidity, dissipationless current flow, and the light-induced exciton spin Hall effect. Here we report on the discovery of interlayer excitons in a bulk van der Waals semiconductor. They form due to strong localization and spin-valley coupling of charge carriers. By combining high-field magneto-reflectance experiments and ab initio calculations for 2H-MoTe2, we explain their salient features: the positive sign of the g-factor and the large diamagnetic shift. Our investigations solve the long-standing puzzle of positive g-factors in transition metal dichalcogenides, and pave the way for studying collective phenomena in these materials at elevated temperatures.

General information
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Organisations: Department of Physics, Theoretical Atomic-scale Physics, University of Munster, CNRS
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A correction to this article has been published and is linked from the HTML version of this article.

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Organisations: Department of Physics, Theoretical Atomic-scale Physics, University of Munster, Laboratoire National de Champs Magnétiques Intenses
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Investigating Catalyst-Support Interactions To Improve the Hydrogen Evolution Reaction Activity of Thiomolybdate [Mo3S13]2- Nanoclusters

Molybdenum sulfides been identified as promising materials for catalyzing the hydrogen evolution reaction (HER) in acid, with active edge sites that exhibit some of the highest turnover frequencies among nonpreciousmetal catalysts. The thiomolybdate [Mo3S13]2- nanocluster catalyst contains a structural motif that resembles the active site of MoS2 and has been reported to be among the most active forms of molybdenum sulfide. Herein, we improve the activity of the [Mo3S13]2- catalysts through catalyst support interactions. We synthesize [Mo3S13]2- on gold, silver, glassy carbon, and copper supports to demonstrate the ability to tune the hydrogen binding energy of [Mo3S13]2- using catalyst support electronic interactions and optimize HER activity.

General information
State: Published
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Pages: 7126-7130
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Publication information
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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
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
**Invisible Trojan-horse attack**

We demonstrate the experimental feasibility of a Trojan-horse attack that remains nearly invisible to the single-photon detectors employed in practical quantum key distribution (QKD) systems, such as Clavis2 from ID Quantique. We perform a detailed numerical comparison of the attack performance against Scarani-Acín-Ribordy-Gisin (SARG04) QKD protocol at 1924 nm versus that at 1536 nm. The attack strategy was proposed earlier but found to be unsuccessful at the latter wavelength, as reported in N. Jain et al., New J. Phys. 16, 123030 (2014). However at 1924 nm, we show experimentally that the noise response of the detectors to bright pulses is greatly reduced, and show by modeling that the same attack will succeed. The invisible nature of the attack poses a threat to the security of practical QKD if proper countermeasures are not adopted.

**General information**

State: Published
Organisations: Department of Physics, Quantum Physics and Information Technology, University of Waterloo
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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
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**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 d⁹ 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 b1g (~x²−y²) and a1g (~3z²−r²) orbitals and also the existence of three nearly equivalent distortions. To clarify this issue we investigate the equilibrium geometry (equatorial, Req, and axial, Rax, Cu²⁺−F⁻ distances) and optical transitions for CuF₆⁴⁻ units formed in Cu²⁺-doped the tetragonal Ba₂ZnF₆ host lattice. While the experimental d-d transitions cannot be reproduced through the isolated CuF₆⁴⁻ unit at the equilibrium geometry, a reasonable agreement is reached adding in the calculation the internal electric field, ER(r), created by the rest of lattice ions on the electrons confined in the complex. It is shown that this tetragonal field, ER(r), already produces a gap Δ₀ ~ 0.35 eV between b1g (~x²−y²) and a1g (~3z²−r²) orbitals of Ba₂ZnF₆:Cu²⁺ when Rax = Req. Nevertheless, as this internal field leads to a Δ₀ 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, ER(r) is shown to be the main physical reason behind an unusual compressed ground state with the hole in the a1g (~3z²−r²) level while it is always placed in the b1g (~x²−y²) level for MX₆ complexes (M = Cu²⁺, Ag²⁺, Ni²⁺; X = F⁻, Cl⁻) in cubic lattices displaying a static JT effect. While the experimental results of CuF₆⁴⁻ in Ba₂ZnF₆ cannot be understood within the JT framework it is pointed out that a quasi-JT situation can however happen for a d⁹ ion in a cubic lattice under a strain of ~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
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BFI (2017): BFI-level 1
Scopus rating (2017): SJR 2.135 SNIP 1.147 CiteScore 4.58
Web of Science (2017): Indexed yes
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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
Josephson Vortex Qubit based on a Confocal Annular Josephson Junction

We report theoretical and experimental work on the development of a Josephson vortex qubit based on a confocal annular Josephson tunnel junction (CAJTJ). The key ingredient of this geometrical configuration is a periodically variable width that generates a spatial vortex potential with bistable states. This intrinsic vortex potential can be tuned by an externally applied magnetic field and tilted by a bias current. The two-state system is accurately modeled by a one-dimensional sine-Gordon like equation by means of which one can numerically calculate both the magnetic field needed to set the vortex in a given state as well as the vortex depinning currents. Experimental data taken at 4.2K on high-quality Nb/Al-AlOx/Nb CAJTJs with an individual trapped fluxon advocate the presence of a robust and finely tunable double-well potential for which reliable manipulation of the vortex state has been classically demonstrated. The vortex is prepared in a given potential by means of an externally applied magnetic field, while the state readout is accomplished by measuring the vortex depinning current in a small magnetic field. Our proof of principle experiment convincingly demonstrates that the proposed vortex qubit based on CAJTJs is robust and workable.

General information
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Organisations: Department of Physics, Institute of Applied Sciences and Intelligent Systems 'E. Caianello', Russian Academy of Sciences
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Layered van der Waals crystals with hyperbolic light dispersion

Compared to artificially structured hyperbolic metamaterials, whose performance is limited by the finite size of the metallic components, the sparse number of naturally hyperbolic materials recently discovered are promising candidates for the next generation of hyperbolic materials. Using first-principles calculations, we extend the number of known naturally hyperbolic materials to the broad class of layered transition metal dichalcogenides (TMDs). The diverse electronic properties of the transition metal dichalcogenides result in a large variation of the hyperbolic frequency regimes ranging from the near-infrared to the ultraviolet. Combined with the emerging field of van der Waals heterostructuring, we demonstrate how the hyperbolic properties can be further controlled by stacking different two-dimensional crystals opening new perspectives for atomic-scale design of photonic metamaterials. As an application, we identify candidates for Purcell factor control of emission from diamond nitrogen-vacancy centers. Natural hyperbolic materials retain the peculiar optical properties of traditional metamaterials whilst not requiring artificial structuring. Here, the authors perform a theoretical screening of a large class of natural materials with hyperbolic dispersion among the family of layered transition metal dichalcogenides.
Ligand manipulation of charge transfer excited state relaxation and spin crossover in $[\text{Fe(2,2'-bipyridine)}_2(\text{CN})_2]$.

We have used femtosecond resolution UV-visible and Kβ x-ray emission spectroscopy to characterize the electronic excited state dynamics of $[\text{Fe(bpy)}_2(\text{CN})_2]$, where bpy=2,2'-bipyridine, initiated by metal-to-ligand charge transfer (MLCT) excitation. The excited-state absorption in the transient UV-visible spectra, associated with the 2,2'-bipyridine radical anion, provides a robust marker for the MLCT excited state, while the transient Kβ x-ray emission spectra provide a clear measure of intermediate and high spin metal-centered excited states. From these measurements, we conclude that the MLCT state of $[\text{Fe(bpy)}_2(\text{CN})_2]$ undergoes ultrafast spin crossover to a metal-centered quintet excited state through a short lived metal-centered triplet transient species. These measurements of $[\text{Fe(bpy)}_2(\text{CN})_2]$ complement prior measurement performed on $[\text{Fe(bpy)}_3]^2^+$ and $[\text{Fe(bpy)}(\text{CN})_4]^{2^-}$ in dimethylsulfoxide solution and help complete the chemical series $[\text{Fe(bpy)}_N(\text{CN})_{6-2N}]^{-2N}$, where $N = 1–3$. The measurements confirm that simple ligand modifications can significantly change the relaxation pathways and excited state lifetimes and support the further investigation of light harvesting and photocatalytic applications of 3d transition metal complexes.

General information
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Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Stanford University, SLAC National Accelerator Laboratory, Deutsches Elektronen-Synchrotron, Lund University, Technical University of Denmark, Max Planck Institute
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Light-Activated Oxidation of the Ligand of an Iron(III) Complex

General information
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Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, University of Groningen, Barcelona Institute of Science and Technology, University of Southern Denmark, The Barcelona Institute of Science and Technology and CSIC
Authors: Wegeberg, C. (Ekstern), Fernández, V. (Ekstern), Frandsen, C. (Intern), Maseras, F. (Ekstern), Browne, W. R. (Ekstern), McKenzie, C. (Ekstern)
Magnetic dipolar ordering and hysteresis of geometrically defined nanoparticle clusters

Magnetic nanoparticle clusters have several biomedical and engineering applications, and revealing the basic interplay between particle configuration and magnetic properties is important for tuning the clusters for specific uses. Here, we consider the nanoparticles as macrospins and use computer simulations to determine their magnetic configuration when placed at the vertices of various polyhedra. We find that magnetic dipoles of equal magnitude arrange in flux-closed vortices on a layer basis, giving the structures a null remanent magnetic moment. Assigning a toroidal moment to each layer, we find that the geometrical arrangement, i.e., “triangular packing” vs. “square packing,” of the moments in the adjacent layer determines whether the flux-closed layers are ferrotoroidal (co-rotating vortices) or antiferrotoroidal (counter-rotating vortices). Interestingly, upon adding a single magnetic moment at the center of the polyhedra, the central moment relaxes along one of the principal axes and induces partial alignment of the surrounding moments. The resulting net moment is up to nearly four times that of the single moment added. Furthermore, we model quasi-static hysteresis loops for structures with and without a central moment. We find that a central moment ensures an opening of the hysteresis loop, and the resultant loop areas are typically many-fold larger compared to the same structure without a central moment.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Center for Electron Nanoscopy
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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
Magnetic order, hysteresis, and phase coexistence in magnetoelectric LiCoPO$_4$

The magnetic phase diagram of magnetoelectric LiCoPO$_4$ is established using neutron diffraction and magnetometry in fields up to 25.9 T applied along the crystallographic b axis. For fields greater than 11.9 T, the magnetic unit cell triples in size with propagation vector $\mathbf{Q} = (0, 1/3, 0)$. A magnetized elliptic cycloid is formed with spins in the (b, c) plane and the major axis oriented along b. Such a structure allows for the magnetoelectric effect with an electric polarization along c induced by magnetic fields applied along b. Intriguingly, additional ordering vectors $\mathbf{Q} \approx (0, 1/4, 0)$ and $\mathbf{Q} \approx (0, 1/2, 0)$ appear for increasing fields in the hysteresis region below the transition field. Traces of this behavior are also observed in the magnetization. A simple model based on a mean-field approach is proposed to explain these additional ordering vectors. In the field interval 20.5-21.0 T, the propagation vector $\mathbf{Q} = (0, 1/3, 0)$ remains but the spins orient differently compared to the cycloid phase. Above 21.0 T and up until saturation, a commensurate magnetic structure exists with a ferromagnetic component along b and an antiferromagnetic component along c.

General information
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Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Technical University of Denmark, Iowa State University, Helmholtz–Zentrum Berlin für Materialien und Energie, Universite Grenoble Alpes, Paul Scherrer Institut, University of Copenhagen
We demonstrate measurements of spectra of O-mode electron cyclotron resonance heating (ECRH) waves scattered collectively from microscopic plasma fluctuations in ASDEX Upgrade discharges with an ITER-like ECRH scenario. The measured spectra are shown to allow determination of the main ion temperature and plasma rotation velocity. This demonstrates that ECRH systems can be exploited for diagnostic purposes alongside their primary heating purpose in a reactor relevant scenario.
Trees present a critical challenge to long-distance transport because as a tree grows in height and the transport pathway increases in length, the hydraulic resistance of the vascular tissue should increase. This has led many to question whether trees can rely on a passive transport mechanism to move carbohydrates from their leaves to their roots. Although species that actively load sugars into their phloem, such as vines and herbs, can increase the driving force for transport as they elongate, it is possible that many trees cannot generate high turgor pressures because they do not use transporters to load sugar into the phloem. Here, we examine how trees can maintain efficient carbohydrate transport as they grow taller by analysing sieve tube anatomy, including sieve plate geometry, using recently developed preparation and imaging techniques, and by measuring the turgor pressures in the leaves of a tall tree in situ. Across nine deciduous species, we find that hydraulic resistance in the phloem scales inversely with plant height because of a shift in sieve element structure along the length of individual trees. This scaling relationship seems robust across multiple species despite large differences in plate anatomy. The importance of this scaling becomes clear when phloem transport is modelled using turgor pressures measured in the leaves of a mature red oak tree. These pressures are of sufficient magnitude to drive phloem transport only in concert with structural changes in the phloem that reduce transport resistance. As a result, the key to the long-standing mystery of how trees maintain phloem transport as they increase in size lies in the structure of the phloem and its ability to change hydraulic properties with plant height.

**Maintenance of carbohydrate transport in tall trees**

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**General information**

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- Authors: Savage, J. A. (Ekstern), Beecher, S. D. (Ekstern), Clerx, L. (Ekstern), Gersony, J. T. (Ekstern), Knoblauch, J. (Ekstern), Losada, J. M. (Ekstern), Jensen, K. H. (Intern), Knoblauch, M. (Ekstern), Holbrook, N. M. (Ekstern)
Manipulating charge transfer excited state relaxation and spin crossover in iron coordination complexes with ligand substitution

Developing light-harvesting and photocatalytic molecules made with iron could provide a cost effective, scalable, and environmentally benign path for solar energy conversion. To date these developments have been limited by the sub-picosecond metal-to-ligand charge transfer (MLCT) electronic excited state lifetime of iron based complexes due to spin crossover—the extremely fast intersystem crossing and internal conversion to high spin metal-centered excited states. We revitalize a 30 year old synthetic strategy for extending the MLCT excited state lifetimes of iron complexes by making mixed ligand iron complexes with four cyanide (CN\(^-\)) ligands and one 2,2’-bipyridine (bpy) ligand. This enables MLCT excited state and metal-centered excited state energies to be manipulated with partial independence and provides a path to suppressing spin crossover. We have combined X-ray Free-Electron Laser (XFEL) Kβ hard X-ray fluorescence spectroscopy with femtosecond time-resolved UV-visible absorption spectroscopy to characterize the electronic excited state dynamics initiated by MLCT excitation of [Fe(CN)\(_4\)(bpy)]\(^2+\). The two experimental techniques are highly complementary; the time-resolved UV-visible measurement probes allowed electronic transitions between valence states making it sensitive to ligand-centered electronic states such as MLCT states, whereas the Kβ fluorescence spectroscopy provides a sensitive measure of changes in the Fe spin state characteristic of metal-centered excited states. We conclude that the MLCT excited state of [Fe(CN)\(_4\)(bpy)]\(^2+\) decays with roughly a 20 ps lifetime without undergoing spin crossover, exceeding the MLCT excited state lifetime of [Fe(2,2’-bipyridine)\(_3\)]\(^2+\) by more than two orders of magnitude.
Manipulation and Motion of Organelles and Single Molecules in Living Cells

The biomolecule is among the most important building blocks of biological systems, and a full understanding of its function forms the scaffold for describing the mechanisms of higher order structures as organelles and cells. Force is a fundamental regulatory mechanism of biomolecular interactions driving many cellular processes. The forces on a molecular scale are exactly in the range that can be manipulated and probed with single molecule force spectroscopy. The natural environment of a biomolecule is inside a living cell, hence, this is the most relevant environment for probing their function. In vivo studies are, however, challenged by the complexity of the cell. In this review, we start with presenting relevant theoretical tools for analyzing single molecule data obtained in intracellular environments followed by a description of state-of-the art visualization techniques. The most commonly used force spectroscopy techniques, namely optical tweezers, magnetic tweezers, and atomic force microscopy, are described in detail, and their strength and limitations related to in vivo experiments are discussed. Finally, recent exciting discoveries within the field of in vivo manipulation and dynamics of single molecule and organelles are reviewed.
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): SNIP 11.97 SJR 23.414 CiteScore 51.08
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 42.79 SJR 19.51 SNIP 10.358
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 18.035 SNIP 11.285 CiteScore 45.92
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 18.38 SNIP 11.392 CiteScore 44.56
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 22.299 SNIP 12.788 CiteScore 49.12
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 20.653 SNIP 11.358 CiteScore 39.08
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 18.613 SNIP 11.05
BFI (2009): BFI-level 2
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 16.304 SNIP 8.663
Web of Science (2008): Indexed yes
Scopus rating (2004): SJR 11.262 SNIP 8.865
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 11.627 SNIP 9.84
Scopus rating (2001): SJR 11.211 SNIP 10.51
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 12.871 SNIP 11.272
Original language: English
Electronic versions:
Untitled.pdf
DOIs:
10.1021/acs.chemrev.6b00638

Bibliographical note
This is an open access article published under an ACS AuthorChoice License
Source: FindIt
Source-ID: 2352219411
Publication: Research - peer-review › Journal article – Annual report year: 2017
McXtrace 1.4: latest developments in the new release
This paper presents details on some of the important new features in the newly released version of the x-ray tracing software package McXtrace. Although many developments have been made, this presentation is focused on the features that were required to meet the challenges posed for accurate simulation of the DanMAX beamline - a beamline currently under design at the MAX IV synchrotron. Among these may be mentioned: new source-models, new monochromator crystal models, multilayer capabilities, and the full beamline simulation frame itself.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Aarhus University
Authors: Knudsen, E. B. (Intern), Willendrup, P. K. (Intern), Garde, J. (Intern), Jørgensen, M. R. V. (Ekstern), Kantor, I. (Intern)
Number of pages: 8
Publication date: 2017

Host publication information
Title of host publication: Proc. SPIE 10403, Infrared Remote Sensing and Instrumentation XXV
Volume: 10388
Publisher: SPIE - International Society for Optical Engineering
Series: Proceedings of SPIE - International Society for Optical Engineering
ISSN: 0277-786X
Main Research Area: Technical/natural sciences
Conference: SPIE Optical Engineering + Applications, San Diego, United States, 06/08/2017 - 06/08/2017
Free electron lasers, Optical simulations, Ray tracing, X-ray, Synchrotrons, Device simulation, Astrophysics
DOIs: 10.1117/12.2274416
Source: FindIt
Source-ID: 2392925013
Publication: Research - peer-review › Article in proceedings – Annual report year: 2017

Measured resolved shear stresses and Bishop-Hill stress states in individual grains of austenitic stainless steel
The full three-dimensional stress state of 172 individual bulk grains in austenitic stainless steel 316L at 0.1 and 1% sample elongation has been determined with sufficient accuracy to allow comparison with the theoretical Bishop-Hill stress states for plastically deforming grains as well as calculation of the resolved shear stresses on the individual slip systems. At 0.1%, the resolved shear stresses exhibit quite large variations between grains of similar orientation. When averaging over similarly oriented grains, the resolved shear stresses correspond to the Schmid factors for uniaxial tension. At 1%, only about half of the grains were close to a Bishop-Hill stress state. The stress state of the other half of the grains was closer to the applied uniaxial stress, in between Bishop-Hill states, or in some cases none of these. The orientation dependence of the assigned stress states deviate somewhat from the theoretical expectation. These deviations are found to originate from a larger tensile stress component than in the theoretical Bishop-Hill stress states and to be associated also with deviations from axisymmetric plastic strain. This conclusion was supported by finite-element crystal plasticity simulations.

General information
State: Published
Organisations: Department of Mechanical Engineering, Materials and Surface Engineering, Department of Physics, Neutrons and X-rays for Materials Physics, University of Illinois at Urbana-Champaign, Cornell High Energy Synchrotron Source, Air Force Research Laboratory
Pages: 388-404
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Acta Materialia
Volume: 141
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
Austenitic stainless steels, Stress and strain, Resolved shear stresses, Synchrotron diffraction, Polycrystal plasticity modelling

Original language: English

DOI: 10.1016/j.actamat.2017.09.021
Mesoporous Ruthenium/Ruthenium Oxide Thin Films: Active Electrocatalysts for the Oxygen Evolution Reaction

We report the first synthesis of a fully contiguous large area supported thin film of highly ordered mesoporous Ru and RuO2 and investigate the electrocatalytic properties towards the oxygen evolution reaction (OER). We find that the nanoscale porous network of these catalysts provides significant enhancements in geometric OER activity without any loss in specific activity. This work demonstrates a strategy for engineering materials at the nanoscale that can simultaneously decrease precious metal loading and increase electrode activity.

General information
State: Published
Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics, SUNCAT Center for Interface Science and Catalysis, Stanford University
Authors: Kibsgaard, J. (Intern), Hellstern, T. R. (Ekstern), Choi, S. (Ekstern), Reinecke, B. N. (Ekstern), Jaramillo, T. F. (Ekstern)
Number of pages: 6
Pages: 2480-2485
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: ChemElectroChem
Volume: 4
Issue number: 10
ISSN (Print): 2196-0216
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 0.727 SJR 1.474 CiteScore 3.94
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
BFI (2013): BFI-level 1
ISI indexed (2013): ISI indexed no
Original language: English
DOIs:
10.1002/celc.201700334
Source: FindIt
Source-ID: 2391817647
Publication: Research - peer-review » Journal article – Annual report year: 2017

Metal-insulator transition in disordered systems from the one-body density matrix

The insulating state of matter can be probed by means of a ground state geometrical marker, which is closely related to the modern theory of polarization (based on a Berry phase). In the present work we show that this marker can be applied to determine the metal-insulator transition in disordered systems. In particular, for noninteracting systems the geometrical marker can be obtained from the configurational average of the norm-squared one-body density matrix, which can be calculated within open as well as periodic boundary conditions. This is in sharp contrast to a classification based on the static conductivity, which is only sensible within periodic boundary conditions. We exemplify the method by considering a simple lattice model, known to have a metal-insulator transition as a function of the disorder strength, and demonstrate that the transition point can be obtained accurately from the one-body density matrix. The approach has a general ab initio formulation and could in principle be applied to realistic disordered materials by standard electronic structure methods.

General information
State: Published
Organisations: Department of Physics, Theoretical Atomic-scale Physics, University of Trieste, Universidad del Pais Vasco
Authors: Olsen, T. (Intern), Resta, R. (Ekstern), Souza, I. (Ekstern)
Number of pages: 6
MeV-range velocity-space tomography from gamma-ray and neutron emission spectrometry measurements at JET

We demonstrate the measurement of a 2D MeV-range ion velocity distribution function by velocity-space tomography at JET. Deuterium ions were accelerated into the MeV-range by third harmonic ion cyclotron resonance heating. We made measurements with three neutron emission spectrometers and a high-resolution γ-ray spectrometer detecting the γ-rays released in two reactions. The tomographic inversion based on these five spectra is in excellent agreement with numerical simulations with the ASCOT–RFOF and the SPOT–RFOF codes. The length of the measured fast-ion tail corroborates the prediction that very few particles are accelerated above 2 MeV due to the weak wave-particle interaction at higher energies.
Micro-CT in situ study of carbonate rock microstructural evolution for geologic CO2 storage

To achieve the 2 degrees C target made in the 2016 Paris Agreement, it is essential to reduce the emission of CO2 into the atmosphere. Carbon Capture and Storage (CCS) has been given increasing importance over the last decade. One of the suggested methods for CCS is to inject CO2 into geologic settings such as the carbonate reservoirs in the North Sea. The final aim of our project is to find out how to control the evolution of petrophysical parameters during CO2 injection using an optimal combination of flow rate, injection pressure and chemical composition of the influent. The first step to achieve this is to find a suitable condition to create a stable 3D space in carbonate rock by injecting liquid to prepare space for the later CO2 injection. Micro-CT imaging is a non-destructive 3D method that can be used to study the property changes of carbonate rocks during and after CO2 injection. The advance in lab source based micro-CT has made it capable of in situ experiments. We used a commercial bench top micro-CT (Zeiss Versa XRM410) to study the microstructure changes of chalk during liquid injection. Flexible temporal CT resolution is essential in this study because that the time scales of coupled physical and chemical processes can be very different. The results validated the feasibility of using a bench top CT system with a pressure cell to monitor the mesoscale multiphase interactions in chalk.

General information

State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, University of Copenhagen
Authors: Zheng, Y. (Intern), Yang, Y. (Ekstern), Rogowska, M. (Ekstern), Gundlach, C. (Intern)
Number of pages: 9
Publication date: 2017
Host publication information
Title of host publication: Proceedings of SPIE
Volume: 10391
Publisher: SPIE - International Society for Optical Engineering
Article number: 103910M
Series: Proceedings of SPIE - International Society for Optical Engineering
Volume: 10391
ISSN: 0277-786X
Main Research Area: Technical/natural sciences
Conference: Developments in X-Ray Tomography XI, San Diego, United States, 08/08/2017 - 08/08/2017
Micro-CT, Porosity, in situ, Oil Reservoir, 4D computed tomography
DOIs: 10.1117/12.2273877
Source: FindIt
Source-ID: 2395822031
Publication: Research - peer-review › Article in proceedings – Annual report year: 2018

Microfabrication of gratings for X-ray phase contrast imaging

General information
State: Published
Organisations: DTU Danchip, Department of Micro- and Nanotechnology, Silicon Microtechnology, Department of Physics, Neutrons and X-rays for Materials Physics, Experimental Surface and Nanomaterials Physics, Technical University of Denmark
Authors: Silvestre, C. (Intern), Hemmingsen, J. H. (Intern), Christensen, E. D. (Forskerdatabase), Kehres, J. (Intern), Hansen, O. (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: H-13
Main Research Area: Technical/natural sciences
Conference: Sustain 2017, Kgs. Lyngby, Denmark, 06/12/2017 - 06/12/2017
Electronic versions: SustainAbstracts2017c.compressed_95.pdf
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2017

Microfabrication of gratings for X-ray Imaging

General information
State: Published
Organisations: DTU Danchip, Department of Micro- and Nanotechnology, Silicon Microtechnology, Department of Physics, Neutrons and X-rays for Materials Physics, Technical University of Denmark
Authors: Silvestre, C. (Intern), Christiansen, E. D. (Ekstern), Zeng, Y. (Ekstern), Kehres, J. (Intern), Jansen, H. (Intern), Hansen, O. (Intern)
Publication date: 2017
Main Research Area: Technical/natural sciences
Electronic versions: Untitled.pdf
Source: PublicationPreSubmission
Source-ID: 137622501
Publication: Research - peer-review › Poster – Annual report year: 2017

Mobilizing industry for ‘big science’
Small- and medium-sized enterprises make good partners for neutron sources and other major research facilities, yet the barriers to entering this market can be high. Nikolaj Zangenberg and Søren Bang Korsholm offer advice on how to overcome them

General information
State: Published
Modeling surface imperfections in thin films and nanostructured surfaces
Accurate scatterometry and ellipsometry characterization of non-perfect thin films and nanostructured surfaces are challenging. Imperfections like surface roughness make the associated modelling and inverse problem solution difficult due to the lack of knowledge about the imperfection on the surface. Combining measurement data from several instruments increases the knowledge of non-perfect surfaces. In this paper we investigate how to incorporate this knowledge of surface imperfection into inverse methods used in scatterometry and ellipsometry using the Rigorous Coupled Wave Analysis. Three classes of imperfections are examined. The imperfections are introduced as periodic structures with a super cell periods ten times larger than the simple grating period. Two classes of imperfections concern the grating and one class concern the substrate. It is shown that imperfections of a few nanometers can severely change the reflective response on silicon gratings. Inverse scatterometry analyses of gratings with imperfection using simulated data with white noise have been performed. The results show that scatterometry is a robust technology that is able to characterize grating imperfections provided that the imperfection class is known.

Modeling the active sites of Co-promoted MoS2 particles by DFT
The atomic-scale structure of the Co-promoted MoS2 catalyst (CoMoS), used for hydrodesulfurization and as a potential replacement for platinum in the acidic hydrogen evolution reaction has been analyzed by modeling its sites using density functional theory and applying thermochemical corrections to account for different reaction conditions. The equilibrium structures of the edges, basal plane and corners have been found and used to obtain a picture of an ideal CoMoS nanoparticle under hydrodesulfurization and hydrogen evolution reaction conditions. Under hydrodesulfurization conditions small energy differences between structures having an additional or missing sulfur atom relative to the equilibrium structures have been observed for the edges and corners explaining their activity towards hydrodesulfurization at the atomic scale. The lack of these small energy differences at the basal plane explains why it is inert towards hydrodesulfurization. The adsorption free energy of hydrogen was calculated and used as a descriptor for qualifying each site in the context of hydrogen evolution, finding that the corner site should perform better than the edges.
Modification of SOL profiles and fluctuations with line-average density and divertor flux expansion in TCV

A set of Ohmic density ramp experiments addressing the role of parallel connection length in modifying scrape off layer (SOL) properties has been performed on the TCV tokamak. The parallel connection length has been modified by varying the poloidal flux expansion $f_x$. It will be shown that this modification does not influence neither the detachment density threshold, nor the development of a flat SOL density profile which instead depends strongly on the increase of the core line average density. The modification of the SOL upstream profile, with the appearance of what is generally called a density shoulder, has been related to the properties of filamentary blobs. Blob size increases with density, without any dependence on the parallel connection length both in the near and far SOL. The increase of the density decay length, corresponding to a profile flattening, has been related to the variation of the divertor normalized collisionality $\Lambda_{\text{div}}$ (Myra et al 2006 Phys. Plasmas 13 112502, Carralero et al, ASDEX Upgrade Team, JET Contributors and EUROfusion MST1 Team 2015 Phys. Rev. Let. 115 215002), showing that in TCV the increase of $\Lambda_{\text{div}}$ is not sufficient to guarantee the SOL upstream profile flattening.

General information

State: Published
Organisations: Department of Physics, Plasma Physics and Fusion Energy, University of Padova, Ecole Polytechnique Federale de Lausanne (EPFL), Culham Science Centre, University of California at San Diego, University of York, University of Innsbruck, FOM Dutch Institute for Fundamental Energy Research , Max Planck Institute for Plasma Physics , Josef Stefan Institute
Number of pages: 14
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Nuclear Fusion
Volume: 57
Issue number: 11
Article number: 116014
ISSN (Print): 0029-5515
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 1.424 SJR 0.759 CiteScore 2.13
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.62 SJR 1.284 SNIP 1.416
Web of Science (2016): Indexed yes
Monte Carlo Particle Lists: MCPL

A binary format with lists of particle state information, for interchanging particles between various Monte Carlo simulation applications, is presented. Portable C code for file manipulation is made available to the scientific community, along with converters and plugins for several popular simulation packages.

Program summary:
Program Title: MCPL.
Nature of problem: Saving particle states in Monte Carlo simulations, for interchange between simulation packages or for reuse within a single package. Solution method: Binary interchange format with associated code written in portable C along with tools and interfaces for relevant simulation packages.

**General information**

State: Published
Organisations: Center for Nuclear Technologies, Radiation Physics, Department of Physics, Neutrons and X-rays for Materials Physics, European Spallation Source ESS AB
Authors: Kittelmann, T. (Ekstern), Klinkby, E. B. (Intern), Bergbäck Knudsen, E. (Intern), Willendrup, P. K. (Intern), Cai, X. X. (Intern), Kanaki, K. (Ekstern)
Number of pages: 26
Pages: 17-42
Publication date: 2017
Main Research Area: Technical/natural sciences

**Publication information**

Journal: Computer Physics Communications
Volume: 218
ISSN (Print): 0010-4655
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 1.999 SJR 1.729 CiteScore 4.19
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.04 SJR 1.914 SNIP 2.094
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.788 SNIP 1.935 CiteScore 3.79
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.344 SNIP 1.649 CiteScore 2.86
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.455 SNIP 1.692 CiteScore 3.17
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.11 SNIP 2.162 CiteScore 3.46
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.75 SNIP 1.951 CiteScore 3.22
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.466 SNIP 1.379
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.228 SNIP 1.266
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.228 SNIP 1.172
Scopus rating (2007): SJR 1.005 SNIP 1.065
Scopus rating (2006): SJR 1.048 SNIP 1.145
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.792 SNIP 1.118
Scopus rating (2004): SJR 1.036 SNIP 1.122
MultiFLEXX - The new multi-analyzer at the cold triple-axis spectrometer FLEXX

The first experimental characterization of a multiple energy analysis wide angle backend for a cold triple-axis spectrometer is reported. The multi-analyzer module MultiFLEXX employs 155 detection channels which simultaneously probe an extensive range in wavevector and energy transfer. Successful mapping of magnetic excitations in MnF$_2$ and Ho demonstrate order of magnitude gains in data collection efficiency using this novel type backend. MultiFLEXX is competitive to standard triple-axis spectroscopy in terms of energy resolution and signal-to-noise ratio. A minority of the detector channels is affected by spurious signals inherent to this multiplexing concept. The characteristic signature of these spurious signals easily allows for their discrimination. The instrument concept focuses on detection efficiency in the horizontal scattering plane which makes it an ideal technique for fast mapping and parametric studies including extreme sample environment.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Ecole Polytechnique Federale de Lausanne (EPFL), Helmholtz–Zentrum Berlin für Materialien und Energie, Technische Universität Dresden, China Institute of Atomic Energy
Authors: Groitl, F. (Ekstern), Toft-Petersen, R. (Intern), Quintero-Castro, D. L. (Ekstern), Meng, S. (Ekstern), Lu, Z. (Ekstern), Huesges, Z. (Ekstern), Le, M. D. (Ekstern), Alimov, S. (Ekstern), Wilpert, T. (Ekstern), Kiefer, K. (Ekstern), Gerischer, S. (Ekstern), Bertin, A. (Ekstern), Habicht, K. (Ekstern)
Number of pages: 12
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Scientific Reports
Volume: 7
Issue number: 1
Article number: 13637
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
Multispectral x-ray CT: multivariate statistical analysis for efficient reconstruction

Recent developments in multispectral X-ray detectors allow for an efficient identification of materials based on their chemical composition. This has a range of applications including security inspection, which is our motivation. In this paper, we analyze data from a tomographic setup employing the MultiX detector, that records projection data in 128 energy bins covering the range from 20 to 160 keV. Obtaining all information from this data requires reconstructing 128 tomograms, which is computationally expensive. Instead, we propose to reduce the dimensionality of projection data prior to reconstruction and reconstruct from the reduced data. We analyze three linear methods for dimensionality reduction using a dataset with 37 equally-spaced projection angles. Four bottles with different materials are recorded for which we are able to obtain similar discrimination of their content using a very reduced subset of tomograms compared to the 128 tomograms that would otherwise be needed without dimensionality reduction.

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Image Analysis & Computer Graphics, Department of Physics, Neutrons and X-rays for Materials Physics
Number of pages: 11
Publication date: 2017

Host publication information
Title of host publication: Proceedings Volume 10391, Developments in X-Ray Tomography XI
Publisher: SPIE - International Society for Optical Engineering
Series: Proceedings of SPIE, the International Society for Optical Engineering
Volume: 1039113
ISSN: 0277-786X
Main Research Area: Technical/natural sciences
Conference: SPIE Optical Engineering + Applications, San Diego, United States, 06/08/2017 - 06/08/2017
DOIs: 10.1117/12.2273338
Source: PublicationPreSubmission
Source-ID: 140806856
Publication: Research - peer-review › Article in proceedings – Annual report year: 2017

Museumstekst og kampen med qi

General information
State: Published
Organisations: Department of Physics
Authors: Zwisler, L. (Intern)
Pages: 28-29
Na-assisted grain growth in CZTS nanoparticle thin films for solar cell applications
We have studied the effect of Na in Cu2ZnSnS4 nanoparticle thin films [1]. The as-synthesized CZTS nanoparticles were inherently ligand-free [2], which allows us to use polar solvents, such as water and ethanol. Another advantage of these particles is that the user- and environmentally-friendly NaCl salt can be directly dissolved in controllable amounts. This further circumvents the need for later incorporation of dopants, or a ligand-exchange step to functionalize the surface of the nanoparticles. In addition, the homogeneous distribution of Na in the ink allows uniform grain growth within the deposited absorber layer. By including Na in the nanoparticle ink, micron-sized grains throughout the whole absorber are achieved after annealing in a sulfur atmosphere at 600°C. The absorber layer appeared to be of full density, and no closed porosity could be detected. In addition, the photoluminescence signal increased by a factor of 200 after Na-inclusion. Without Na, the grains were very difficult to sinter, the film was porous, and the photoluminescence was low. A concentration of Na/(Cu+Zn+Sn)=30% was necessary for the densification of the absorber, which is significantly higher than that used in other Na-doped CZTS systems. The annealed films were found to be of the desired Cu-poor and Zn-rich composition. We also found that a sulfidation temperature above 550°C was required. At 550°C, NaCl-crystals appeared on the surface of the thin films, suggesting an incomplete transformation of Na into the liquid phase Na2Sx-additive during sintering. At this temperature, grain growth was only detected in close proximity to the NaCl regions. It was also observed that the NaCl crystals could be easily removed by a quick water rinse, but that this treatment reduced the photoluminescence signal. This is relevant as it is customary to leave the absorber layer in a water-based solution after annealing before buffer layer deposition.

Narrow-bandwidth sensing of high-frequency fields with continuous dynamical decoupling
State-of-the-art methods for sensing weak AC fields are only efficient in the low frequency domain (<10 MHz). The inefficiency of sensing high-frequency signals is due to the lack of ability to use dynamical decoupling. In this paper we show that dynamical decoupling can be incorporated into high-frequency sensing schemes and by this we demonstrate that the high sensitivity achieved for low frequency can be extended to the whole spectrum. While our scheme is general and suitable to a variety of atomic and solid-state systems, we experimentally demonstrate it with the nitrogen-vacancy center in diamond. For a diamond with natural abundance of 13C, we achieve coherence times up to 1.43 ms resulting in a smallest detectable magnetic field strength of 4 nT at 1.6 GHz. Attributed to the inherent nature of our scheme, we observe an additional increase in coherence time due to the signal itself.
New Platinum Alloy Catalysts for Oxygen Electroreduction Based on Alkaline Earth Metals

The energy efficiency of polymer electrolyte membrane fuel cells is mainly limited by overpotentials related to the oxygen reduction reaction (ORR). In this paper, we present new platinum alloys which are active for the ORR and based on alloying Pt with very abundant elements, such as Ca. Theoretical calculations suggested that Pt$_5$Ca and Pt$_5$Sr should be active for the ORR. Electrochemical measurements show that the activity of sputter-cleaned polycrystalline Pt$_5$Ca and Pt$_5$Sr electrodes is enhanced by a factor of 5–7 relative to polycrystalline Pt. Accelerated stability testing shows that after 10,000 electrochemical cycles, the alloys still retain over half their activity. The stability is thus not quite on par with the similar Pt-lanthanide alloys, possibly due to the somewhat lower heat of formation.

General information
State: Published
Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics, Theoretical Atomic-scale Physics, University of Copenhagen
Number of pages: 11
Pages: 594-604
Publication date: 2017
Main Research Area: Technical/natural sciences
Nitrogen-vacancy ensemble magnetometry based on pump absorption
We demonstrate magnetic field sensing by recording the variation in the pump light absorption with nitrogen-vacancy center ensemble. At a frequency of 10 mHz we obtain a noise floor of ~30 nT/√Hz.
Numerical simulations of blobs with ion dynamics

The transport of particles and energy into the scrape-off layer (SOL) region at the outboard midplane of medium-sized tokamaks, operating in low confinement mode, is investigated by applying the first-principle HESEL (hot edge-sol-electrostatic) model. HESEL is a four-field drift-fluid model including finite electron and ion temperature effects, drift wave dynamics on closed field lines, and sheath dynamics on open field lines. Particles and energy are mainly transported by intermittent blobs. Therefore, blobs have a significant influence on the corresponding profiles. The formation of a 'shoulder' in the SOL density profile can be obtained by increasing the collisionality or connection length, thus decreasing the efficiency of the SOL's ability to remove plasma. As the ion pressure has a larger perpendicular but smaller parallel dissipation rate compared to the electron pressure, ion energy is transported far into the SOL. This implies that the ion temperature in the SOL exceeds the electron temperature by a factor of 2-4 and significantly broadens the power deposition profile.

General information
State: Published
Organisations: Department of Physics, Plasma Physics and Fusion Energy, Chinese Academy of Sciences, Technical University of Denmark
Authors: Nielsen, A. H. (Intern), Rasmussen, J. J. (Intern), Madsen, J. (Intern), Xu, G. S. (Ekstern), Naulin, V. (Intern), Olsen, J. M. B. (Intern), Magnussen, M. L. (Intern), Hansen, S. (Ekstern), Yan, N. (Ekstern), Tophøj, L. E. H. (Intern), Wan, B. N. (Ekstern)
Number of pages: 12
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Plasma Physics and Controlled Fusion
Volume: 59
Issue number: 2
Article number: 025012
ISSN (Print): 0741-3335
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 1.243 SJR 0.69 CiteScore 1.74
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1 SJR 1.433 SNIP 1.258
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.314 SNIP 1.345 CiteScore 1.1
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.542 SNIP 1.346 CiteScore 1.61
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.2 SNIP 1.253 CiteScore 1.54
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.453 SNIP 1.201 CiteScore 1.63
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.496 SNIP 1.591 CiteScore 2.69
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Observation of short time-scale spectral emissions at millimeter wavelengths with the new CTS diagnostic on the FTU tokamak: Paper

On the FTU tokamak, the collective Thomson scattering (CTS) diagnostic was renewed for investigating the possible excitation of parametric decay instabilities (PDI) by electron cyclotron (EC) or CTS probe beams in presence of magnetic islands and measure their effects on the EC power absorption. The experiments were performed launching a gyrotron probe beam (140 GHz, 400 kW) and observing the scattered radiation in symmetric and asymmetric directions (with respect to the equatorial plane) in different conditions of plasma density and magnetic field (with or without the EC resonance in the plasma), and with magnetic islands generated by Neon injection. The acquisition with a fast digitizer allowed observing spectral features with very high time and frequency resolution. Shots were performed at 7.2 T, with the fundamental EC resonance out of the plasma region, at 4.7 T, with the resonance on the high field side of the plasma column, and at 3.6 T, in this last case with the plasma between the first and the second EC harmonics both lying outside the plasma volume. Several types of spectral features characterized by their frequency and their fast time evolution were identified in the observed signal after a proper treatment. The paper reports the observations in the different experimental cases and the correlation of the features with the existence of MHD modes as witnessed by magnetic probes signals and with macroscopic plasma parameters.

General information

State: Published
Organisations: Department of Physics, Plasma Physics and Fusion Energy, Consiglio Nazionale delle Ricerche, ENEA Centro Ricerche Frascati, Ecole Polytechnique Federale de Lausanne (EPFL), RAS - Institute of Applied Physics, Università degli Studi di Milano-Bicocca, Università degli Studi di Napoli Federico II
Authors: Bruschi, A. (Ekstern), Alessi, E. (Ekstern), Bin, W. (Ekstern), D'Arcangelo, O. (Ekstern), Baiocchi, B. (Ekstern), Belli, F. (Ekstern), Calabro, G. (Ekstern), Casiraghi, I. (Ekstern), Cocilovo, V. (Ekstern), Figini, L. (Ekstern), Galperti, C. (Ekstern), Garavaglia, S. (Ekstern), Granucci, G. (Ekstern), Grosso, G. (Ekstern), Korsholm, S. B. (Intern), Lontano, M. (Ekstern), Mazzotta, C. (Ekstern), Mollera, V. (Ekstern), Del Moro, A. (Ekstern), Nielsen, S. K. (Intern), Orsito, F. (Ekstern), Pedersen, M. S. (Intern), Tartari, U. (Ekstern)
Number of pages: 8
Publication date: 2017
Main Research Area: Technical/natural sciences
Off-axis spin orientation in goethite nanoparticles

Neutron diffraction is a powerful technique for determining the magnetic structure of antiferromagnetic materials. However, for some of these, determining the detailed magnetic structure remains a challenge. In goethite (α-FeOOH) the antiferromagnetic unit cell coincides with the chemical unit cell and, consequently, nuclear and magnetic diffraction peaks occur at the same positions. Analysis of diffraction data from goethite is further complicated by finite-size peak broadening, resulting from goethite commonly occurring in nanocrystalline form. For these reasons, determining the magnetic structure of goethite has been challenging, and few detailed studies have been published. Even today, not all aspects of the magnetic structure are well established. Here, we investigate the magnetic structure of three samples of goethite nanoparticles with polarized neutron powder diffraction (xyz-polarization analysis). Two samples consist of acicular goethite particles that are approximately 40 nm long and with different thicknesses, and one sample consists of pseudospherical particles with a diameter of approximately 5 nm. The larger particles consist of several crystallites whereas the 5-nm particles are mostly single crystalline. The polarization analysis enables us to separate magnetic scattering from nuclear and spin-incoherent scattering, resulting in data that can readily be analyzed. For the two samples with the larger particle size, we find nuclear correlation lengths in the [100] direction that are approximately 3 nm longer than the magnetic correlation lengths, indicating a magnetically disordered layer perpendicular to the antiferromagnetic modulation direction. We find no evidence of a magnetically disordered surface layer in the 5-nm particles. We find the magnetic structure to be antiferromagnetic but, in contrast to most previous studies, we find the spin orientation in all three samples to make an angle of 28-30° with respect to the crystallographic b axis.
On the analysis of time-of-flight spin-echo modulated dark-field imaging data
Spin-Echo Modulated Small Angle Neutron Scattering with spatial resolution, i.e. quantitative Spin-Echo Dark Field Imaging, is an emerging technique coupling neutron imaging with spatially resolved quantitative small angle scattering information. However, the currently achieved relatively large modulation periods of the order of millimeters are superimposed to the images of the samples. So far this required an independent reduction and analyses of the image and scattering information encoded in the measured data and is involving extensive curve fitting routines. Apart from requiring a priori decisions potentially limiting the information content that is extractable also a straightforward judgment of the data quality and information content is hindered. In contrast we propose a significantly simplified routine directly applied to the measured data, which does not only allow an immediate first assessment of data quality and delaying decisions on potentially information content limiting further reduction steps to a later and better informed state, but also, as results suggest, generally better analyses. In addition the method enables to drop the spatial resolution detector requirement for non-spatially resolved Spin-Echo Modulated Small Angle Neutron Scattering.

General information
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Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Delft University of Technology, University of Copenhagen, Helmholtz–Zentrum Berlin für Materialien und Energie, University of California at Berkeley
Authors: Sales, M. (Intern), Plomp, J. (Ekstern), Bouwman, W. G. (Ekstern), Tremsin, A. S. (Ekstern), Habicht, K. (Ekstern), Strobl, M. (Ekstern)
Number of pages: 10
Pages: 012026
On the ‘centre of gravity’ method for measuring the composition of magnetite/maghemite mixtures, or the stoichiometry of magnetite-maghemite solid solutions, via 57Fe Mössbauer spectroscopy

We evaluate the application of 57Fe Mössbauer spectroscopy to the determination of the composition of magnetite (Fe3O4)/maghemite (γ-Fe2O3) mixtures and the stoichiometry of magnetite-maghemite solid solutions. In particular, we consider
a recently proposed model-independent method which does not rely on a priori assumptions regarding the nature of the sample, other than that it is free of other Fe-containing phases. In it a single parameter, δ̅RT-the 'centre of gravity', or area weighted mean isomer shift at room temperature, T = 295 ± 5 K-is extracted by curve-fitting a sample’s Mössbauer spectrum, and is correlated to the sample’s composition or stoichiometry. We present data on high-purity magnetite and maghemite powders, and mixtures thereof, as well as comparison literature data from nanoparticulate mixtures and solid solutions, to show that a linear correlation exists between δ̅RT and the numerical proportion of Fe atoms in the magnetite environment: a = Fe_{magnetite}/Fe_{total} = (δ̅RT - δo)/m, where δo = 0.3206 ± 0.0022 mm s^{-1} and m = 0.2135 ± 0.0076 mm s^{-1}. We also present equations to relate a to the weight percentage w of magnetite in mixed phases, and the magnetite stoichiometry x = Fe^{2+}/Fe^{3+} in solid solutions. The analytical method is generally applicable, but is most accurate when the absorption profiles are sharp; in some samples this may require spectra to be recorded at reduced temperatures. We consider such cases and provide equations to relate δ(T) to the corresponding a value.

General information
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Organisations: Department of Micro- and Nanotechnology, Magnetic Systems, Department of Physics, Neutrons and X-rays for Materials Physics, University College London, Universidad de Cantabria
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Web of Science (2017): Indexed yes
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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
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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
On the elusive crystal structure of expanded austenite

No consistent structural description exists for expanded austenite that accurately accounts for the hkl-dependent peak shifts and broadening observed in diffraction experiments. The best available description for homogeneous samples is a face-centered cubic lattice with stacking faults. Here Debye simulations of stacking fault effects were compared to experimental data for macro-stress free homogeneous expanded austenite to show that a faulted structure cannot explain the observed peak displacement anomalies. Instead it is argued that the shifts are the combined result of elastic and plastic anisotropy leading to (strongly) non-linear hkl-dependent elastic behavior during composition-induced plastic deformation on synthesis of expanded austenite.

General information
State: Published
Organisations: Department of Mechanical Engineering, Materials and Surface Engineering, Department of Physics, Neutrons and X-rays for Materials Physics, Department of Chemistry, X-ray Crystallography
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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
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 2.314 SNIP 2.082 CiteScore 3.21
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 2.427 SNIP 2.117
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.569 SNIP 1.999
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 2.607 SNIP 2.108
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 2.216 SNIP 2.157
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 2.079 SNIP 1.899
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.877 SNIP 1.885
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.584 SNIP 1.679
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.622 SNIP 1.687
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 1.603 SNIP 1.338
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 1.26 SNIP 1.345
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Scopus rating (2000): SJR 1.61 SNIP 1.102
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 1.476 SNIP 1.151
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On the instabilities of a potential vortex with a free surface

In this paper, we address the linear stability analysis of a confined potential vortex with a free surface. This particular flow has been recently used by Tophøj et al. (Phys. Rev. Lett., vol. 110(19), 2013, article 194502) as a model for the swirling flow of fluid in an open cylindrical container, driven by rotating the bottom plate (the rotating bottom experiment) to explain the so-called rotating polygons instability (Vatistas J. Fluid Mech., vol. 217, 1990, pp. 241-248; Jansson et al., Phys. Rev. Lett., vol. 96, 2006, article 174502) in terms of surface wave interactions leading to resonance. Global linear stability results are complemented by a Wentzel-Kramers-Brillouin-Jeffreys (WKBJ) analysis in the shallow-water limit as well as new experimental observations. It is found that global stability results predict additional resonances that cannot be captured by the simple wave coupling model presented in Tophøj et al. (2013). Both the main resonances (thought to be at the root of the rotating polygons) and these secondary resonances are interpreted in terms of over-reflection phenomena by the WKBJ analysis. Finally, we provide experimental evidence for a secondary resonance supporting the numerical and theoretical analysis presented. These different methods and observations allow to support the unstable wave coupling mechanism as the physical process at the origin of the polygonal patterns observed in free-surface rotating flows.

General information
State: Published
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Scopus rating (2017): SJR 1.591 SNIP 1.702 CiteScore 3.33
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BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.82 SJR 1.744 SNIP 1.671
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.896 SNIP 1.639 CiteScore 2.57
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.864 SNIP 1.805 CiteScore 2.66
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.853 SNIP 1.88 CiteScore 2.71
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.678 SNIP 1.86 CiteScore 2.47
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 2.059 SNIP 2.002 CiteScore 2.72
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Operando investigation of Au-MnOx thin films with improved activity for the oxygen evolution reaction

The electrochemical splitting of water holds great potential as a method for producing clean fuels by storing electricity from intermittent energy sources. The efficiency of such a process would be greatly facilitated by incorporating more active catalysts based on abundant materials for the oxygen evolution reaction. Manganese oxides are promising as catalysts for this reaction. Recent reports show that their activity can be drastically enhanced when modified with gold. Herein, we investigate highly active mixed Au-MnOx thin films for the oxygen evolution reaction, which exhibit more than five times improvement over pure MnOx. These films are characterized with operando X-ray Absorption Spectroscopy, which reveal that Mn assumes a higher oxidation state under reaction conditions when Au is present. The magnitude of the enhancement is correlated to the size of the Au domains, where larger domains are the more beneficial.
Optical and hydrodynamic stretching of single cells from blood

Mechanical properties, like deformability or elasticity, of cells can in some cases be indicative of the health of the organism they originate from. In this work, we explore the potential of deformability and other mechanical parameters of individual red blood cells (RBCs) from humans as a marker for the state of health of the human source, patient or donor. In particular, we have investigated the use of different experimental strategies implemented in injection molded plastic microfluidic devices. One strategy is to optically stretch the red blood cells in an optical two-beam trap, also known as an optical stretcher, in a microfluidic chip in which optical fibers have been placed during a post-processing step. Another strategy is to exert hydrodynamic shear forces on the cells by forcing the cells through a narrow constriction. The latter method has the advantage of a considerably higher throughput but does so far not allow for subsequent investigations of single "interesting" cells. The paper is a progress report with preliminary results based on the different strategies, we have pursued.

Optical simulations for design, alignment, and performance prediction of silicon pore optics for the ATHENA x-ray telescope

The ATHENA X-ray observatory is a large-class ESA approved mission, with launch scheduled in 2028. The technology of silicon pore optics (SPO) was selected as baseline to assemble ATHENA’s optic with hundreds of mirror modules, obtained by stacking wedged and ribbed silicon wafer plates onto silicon mandrels to form the Wolter-I configuration. In the current configuration, the optical assembly has a 3 m diameter and a 2 m2 effective area at 1 keV, with a required angular resolution of 5 arcsec. The angular resolution that can be achieved is chiefly the combination of 1) the focal spot size determined by the pore diffraction, 2) the focus degradation caused by surface and profile errors, 3) the aberrations introduced by the misalignments between primary and secondary segments, 4) imperfections in the co-focality of the mirror modules in the optical assembly. A detailed simulation of these aspects is required in order to assess the fabrication and alignment tolerances; moreover, the achievable effective area and angular resolution depend on the mirror module design. Therefore, guaranteeing these optical performances requires: a fast design tool to find the most performing solution in terms of mirror module geometry and population, and an accurate point spread function simulation from local metrology and positioning information. In this paper, we present the results of simulations in the framework of ESA-financed projects (SIMPOSiuM, ASPHEA, SPIRIT), in preparation of the ATHENA X-ray telescope, analyzing the mentioned points: 1) we deal with a detailed description of diffractive effects in an SPO mirror module, 2) we show ray-tracing results including surface and profile defects of the reflective surfaces, 3) we assess the effective area and angular resolution degradation caused by alignment errors between SPO mirror module segments, and 4) we simulate the effects of co-focality errors in X-rays and in the UV optical bench used to study the mirror module alignment and integration.
Optics for electron cyclotron resonance heating and collective Thomson scattering at the stellarator W7-X

This paper will provide a brief review on the optical transmission system, describe its performance and first experiences, and will concentrate on new developments like in-vessel grating reflectors, Remote-steering (RS) antennas used as launchers and receivers for ECRH and collective Thomson scattering (CTS), as well as possible upgrades.
Optimally cloned binary coherent states

Binary coherent state alphabets can be represented in a two-dimensional Hilbert space. We capitalize this formal connection between the otherwise distinct domains of qubits and continuous variable states to map binary phase-shift keyed coherent states onto the Bloch sphere and to derive their quantum-optimal clones. We analyze the Wigner function and the cumulants of the clones, and we conclude that optimal cloning of binary coherent states requires a nonlinearity above second order. We propose several practical and near-optimal cloning schemes and compare their cloning fidelity to the optimal cloner.

General information
State: Published
Organisations: Department of Physics, Quantum Physics and Information Technology, Max Planck Institute for the Science of Light
Authors: Mueller, C. R. (Ekstern), Leuchs, G. (Ekstern), Marquardt, C. (Ekstern), Andersen, U. L. (Intern)
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Web of Science (2017): Indexed yes
Scopus rating (2016): CiteScore 2.25 SJR 1.482 SNIP 0.985
Web of Science (2016): Indexed yes
Scopus rating (2015): SJR 1.747 SNIP 1.008 CiteScore 2.06
Web of Science (2015): Indexed yes
Scopus rating (2014): SJR 2.201 SNIP 1.163 CiteScore 2.46
Web of Science (2014): Indexed yes
Scopus rating (2013): SJR 2.305 SNIP 1.166 CiteScore 2.86
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Scopus rating (2012): SJR 2.519 SNIP 1.231 CiteScore 2.81
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Web of Science (2012): Indexed yes
Scopus rating (2011): SJR 2.316 SNIP 1.252 CiteScore 2.79
Optimised frequency modulation for continuous-wave optical magnetic resonance sensing using nitrogen-vacancy ensembles

Magnetometers based on ensembles of nitrogen-vacancy centres are a promising platform for continuously sensing static and low-frequency magnetic fields. Their combination with phase-sensitive (lock-in) detection creates a highly versatile sensor with a sensitivity that is proportional to the derivative of the optical magnetic resonance lock-in spectrum, which is in turn dependant on the lock-in modulation parameters. Here we study the dependence of the lock-in spectral slope on the modulation of the spin-driving microwave field. Given the presence of the intrinsic nitrogen hyperfine spin transitions, we experimentally show that when the ratio between the hyperfine linewidth and their separation is ≥ 1/4, square-wave based frequency modulation generates the steepest slope at modulation depths exceeding the separation of the hyperfine lines, compared to sine-wave based modulation. We formulate a model for calculating lock-in spectra which shows excellent agreement with our experiments, and which shows that an optimum slope is achieved when the linewidth/separation ratio is ≥ 1/4 and the modulation depth is less than the resonance linewidth, irrespective of the modulation function used.

General information
State: Published
Organisations: Department of Physics, Quantum Physics and Information Technology
Authors: El-Ella, H. (Intern), Ahmadi, S. (Intern), Wojciechowski, A. (Intern), Huck, A. (Intern), Andersen, U. L. (Intern)
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Main Research Area: Technical/natural sciences
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

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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
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Main Research Area: Technical/natural sciences

Overview of ASDEX Upgrade results

The ASDEX Upgrade (AUG) programme is directed towards physics input to critical elements of the ITER design and the preparation of ITER operation, as well as addressing physics issues for a future DEMO design. Since 2015, AUG is equipped with a new pair of 3-strap ICRF antennas, which were designed for a reduction of tungsten release during ICRF operation. As predicted, a factor two reduction on the ICRF-induced W plasma content could be achieved by the reduction of the sheath voltage at the antenna limiters via the compensation of the image currents of the central and side straps in the antenna frame. There are two main operational scenario lines in AUG. Experiments with low collisionality, which comprise current drive, ELM mitigation/suppression and fast ion physics, are mainly done with freshly boronized walls to reduce the tungsten influx at these high edge temperature conditions. Full ELM suppression and non-inductive operation up to a plasma current of $I_p = 0.8$ MA could be obtained at low plasma density. Plasma exhaust is studied under conditions of high neutral divertor pressure and separatrix electron density, where a fresh boronization is not required. Substantial progress could be achieved for the understanding of the confinement degradation by strong D puffing and the improvement with nitrogen or carbon seeding. Inward/outward shifts of the electron density profile relative to the temperature profile affect the edge stability via the pressure profile changes and lead to improved/decreased pedestal performance. Seeding and D gas puffing are found to effect the core fueling via changes in a region of high density on the high field side (HFSHD). The integration of all above mentioned operational scenarios will be feasible and naturally
obtained in a large device where the edge is more opaque for neutrals and higher plasma temperatures provide a lower collisionality. The combination of exhaust control with pellet fueling has been successfully demonstrated. High divertor enrichment values of nitrogen $E^N_N \geq 10$ have been obtained during pellet injection, which is a prerequisite for the simultaneous achievement of good core plasma purity and high divertor radiation levels. Impurity accumulation observed in the all-metal AUG device caused by the strong neoclassical inward transport of tungsten in the pedestal is expected to be relieved by the higher neoclassical temperature screening in larger devices.

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Scopus rating (2017): SNIP 1.424 SJR 0.759 CiteScore 2.13
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.62 SJR 1.284 SNIP 1.416
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.51 SNIP 1.62 CiteScore 1.88
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.907 SNIP 1.667 CiteScore 2.2
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.366 SNIP 1.516 CiteScore 1.83
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.441 SNIP 1.448 CiteScore 1.81
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.043 SNIP 2.433 CiteScore 3.78
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 2.268 SNIP 1.927
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.993 SNIP 2.441
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Overview of progress in European medium sized tokamaks towards an integrated plasma-edge/wall solution

Integrating the plasma core performance with an edge and scrape-off layer (SOL) that leads to tolerable heat and particle loads on the wall is a major challenge. The new European medium size tokamak task force (EU-MST) coordinates research on ASDEX Upgrade (AUG), MAST and TCV. This multi-machine approach within EU-MST, covering a wide parameter range, is instrumental to progress in the field, as ITER and DEMO core/pedestal and SOL parameters are not achievable simultaneously in present day devices. A two prong approach is adopted. On the one hand, scenarios with tolerable transient heat and particle loads, including active edge localised mode (ELM) control are developed. On the other hand, divertor solutions including advanced magnetic configurations are studied. Considerable progress has been made on both approaches, in particular in the fields of: ELM control with resonant magnetic perturbations (RMP), small ELM regimes, detachment onset and control, as well as filamentary scrape-off-layer transport. For example full ELM suppression has now been achieved on AUG at low collisionality with n=2 RMP maintaining good confinement $H_{\alpha}(98,y^2) =0.95$ Advances have been made with respect to detachment onset and control. Studies in advanced divertor configurations (Snowflake, Super-X and X-point target divertor) shed new light on SOL physics. Cross field filamentary transport has been characterised in a wide parameter regime on AUG, MAST and TCV progressing the theoretical and experimental understanding crucial for predicting first wall loads in ITER and DEMO. Conditions in the SOL also play a crucial role for ELM stability and access to small ELM regimes.

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Organisations: Department of Physics, Plasma Physics and Fusion Energy, Technical University of Denmark
Overview of recent physics results from MAST

New results from MAST are presented that focus on validating models in order to extrapolate to future devices. Measurements during start-up experiments have shown how the bulk ion temperature rise scales with the square of the reconnecting field. During the current ramp-up, models are not able to correctly predict the current diffusion. Experiments have been performed looking at edge and core turbulence. At the edge, detailed studies have revealed how filament characteristics are responsible for determining the near and far scrape off layer density profiles. In the core the intrinsic rotation and electron scale turbulence have been measured. The role that the fast ion gradient has on redistributing fast ions through fishbone modes has led to a redesign of the neutral beam injector on MAST Upgrade. In H-mode the turbulence at the pedestal top has been shown to be consistent with being due to electron temperature gradient modes. A reconnection process appears to occur during edge localized modes (ELMs) and the number of filaments released determines the power profile at the divertor. Resonant magnetic perturbations can mitigate ELMs provided the edge peeling response is maximised and the core kink response minimised. The mitigation of intrinsic error fields with toroidal mode number n > 1 has been shown to be important for plasma performance.

General information
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Organisations: Plasma Physics and Fusion Energy, Department of Physics

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Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.62 SJR 1.284 SNIP 1.416
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.51 SNIP 1.62 CiteScore 1.88
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.907 SNIP 1.667 CiteScore 2.2
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.366 SNIP 1.516 CiteScore 1.83
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.441 SNIP 1.448 CiteScore 1.81
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.043 SNIP 2.433 CiteScore 3.78
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 2.268 SNIP 1.927
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.993 SNIP 2.441
Overview of the JET results in support to ITER

The 2014–2016 JET results are reviewed in the light of their significance for optimising the ITER research plan for the active and non-active operation. More than 60 h of plasma operation with ITER first wall materials successfully took place since its installation in 2011. New multi-machine scaling of the type I-ELM divertor energy flux density to ITER is supported by first principle modelling. ITER relevant disruption experiments and first principle modelling are reported with a set of three disruption mitigation valves mimicking the ITER setup. Insights of the L–H power threshold in Deuterium and Hydrogen are given, stressing the importance of the magnetic configurations and the recent measurements of fine-scale structures in the edge radial electric. Dimensionless scans of the core and pedestal confinement provide new information to elucidate the importance of the first wall material on the fusion performance. H-mode plasmas at ITER triangularity (H = 1 at βN ~ 1.8 and n/nGW ~ 0.6) have been sustained at 2 MA during 5 s. The ITER neutronics codes have been validated on high performance experiments. Prospects for the coming D–T campaign and 14 MeV neutron calibration strategy are reviewed.

General information

State: Published
Organisations: Department of Informatics and Mathematical Modeling, Department of Physics, Plasma Physics and Fusion Energy
Overview of the TCV tokamak program: scientific progress and facility upgrades

The TCV tokamak is augmenting its unique historical capabilities (strong shaping, strong electron heating) with ion heating, additional electron heating compatible with high densities, and variable divertor geometry, in a multifaceted upgrade program designed to broaden its operational range without sacrificing its fundamental flexibility. The TCV program is rooted in a three-pronged approach aimed at ITER support, explorations towards DEMO, and fundamental research. A 1 MW, tangential neutral beam injector (NBI) was recently installed and promptly extended the TCV parameter range, with record ion temperatures and toroidal rotation velocities and measurable neutral-beam current drive. ITER-relevant scenario development has received particular attention, with strategies aimed at maximizing performance through optimized discharge trajectories to avoid MHD instabilities, such as peeling-ballooning and neoclassical tearing modes. Experiments on exhaust physics have focused particularly on detachment, a necessary step to a DEMO reactor, in a comprehensive set of conventional and advanced divertor concepts. The specific theoretical prediction of an enhanced radiation region between the two X-points in the low-field-side snowflake-minus configuration was experimentally confirmed. Fundamental investigations of the power decay length in the scrape-off layer (SOL) are progressing rapidly, again in widely varying configurations and in both D and He plasmas; in particular, the double decay length in L-mode limited plasmas was found to be replaced by a single length at high SOL resistivity. Experiments on disruption mitigation by massive gas injection and electron-cyclotron resonance heating (ECRH) have begun in earnest, in parallel with studies of runaway electron generation and control, in both stable and disruptive conditions; a quiescent runaway beam carrying the entire electrical current appears to develop in some cases. Developments in plasma control have benefited from progress in individual controller design and have evolved steadily towards controller integration, mostly within an environment supervised by a tokamak profile control simulator. TCV has demonstrated effective wall conditioning with ECRH in He in support of the preparations for JT-60SA operation.
Parametric decay instability near the upper hybrid resonance and anomalous mm-wave scattering in tokamak and stellarator plasmas

General information
State: Published
Organisations: Department of Physics, Plasma Physics and Fusion Energy, Max-Planck-Institut fur Plasmaphysik, Technical University of Denmark
Authors: Hansen, S. K. (Ekstern), Nielsen, S. K. (Intern), Salewski, M. (Intern), Pedersen, M. S. (Intern), Stober, J. (Ekstern), Team, A. U. (Ekstern)
Number of pages: 2
Publication date: 2017
Conference: 10th International Workshop 2017 "Strong Microwaves and Terahertz Waves: Sources and Applications", Moscow, Russian Federation, 17/07/2017 - 17/07/2017
Main Research Area: Technical/natural sciences

Publication information
In this paper we investigate parametric decay of an electromagnetic pump wave into two electrostatic daughter waves, particularly an X-mode pump wave decaying into a warm upper hybrid wave (a limit of an electron Bernstein wave) and a warm lower hybrid wave. We describe the general theory of the above parametric decay instability (PDI), unifying earlier treatments, and show that it may occur in underdense and weakly overdense plasmas. The PDI theory is used to explain anomalous sidebands observed in collective Thomson scattering (CTS) spectra at the ASDEX Upgrade tokamak. The theory may also account for similar observations during CTS experiments in stellarators, as well as in some 1st harmonic electron cyclotron resonance and O-X-B heating experiments.
Passive phloem loading and long-distance transport in a synthetic tree-on-a-chip

Vascular plants rely on differences in osmotic pressure to export sugars from regions of synthesis (mature leaves) to sugar sinks (roots, fruits). In this process, known as Münch pressure flow, the loading of sugars from photosynthetic cells to the export conduit (the phloem) is crucial, as it sets the pressure head necessary to power long-distance transport. Whereas most herbaceous plants use active mechanisms to increase phloem sugar concentration above that of the photosynthetic cells, in most tree species, for which transport distances are largest, loading seems, counterintuitively, to occur by means of passive symplastic diffusion from the mesophyll to the phloem. Here, we use a synthetic microfluidic model of a passive loader to explore the non-linear dynamics that arise during export and determine the ability of passive...
loading to drive long-distance transport. We first demonstrate that in our device, the phloem concentration is set by the balance between the resistances to diffusive loading from the source and convective export through the phloem. Convection-limited export corresponds to classical models of Münch transport, where the phloem concentration is close to that of the source; in contrast, diffusion-limited export leads to small phloem concentrations and weak scaling of flow rates with hydraulic resistance. We then show that the effective regime of convection-limited export is predominant in plants with large transport resistances and low xylem pressures. Moreover, hydrostatic pressures developed in our synthetic passive loader can reach botanically relevant values as high as 10 bars. We conclude that passive loading is sufficient to drive long-distance transport in large plants, and that trees are well suited to take full advantage of passive phloem loading strategies.

General information
State: Published
Organisations: Department of Physics, Biophysics and Fluids, Massachusetts Institute of Technology, Cornell University
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Publication date: 2017
Main Research Area: Technical/natural sciences

Performance Study of Acoustophoretic Microfluidic Silicon-Glass Devices by Characterization of Material- and Geometry-Dependent Frequency Spectra
The mechanical and electrical response of acoustophoretic microfluidic devices attached to an ac-voltage-driven piezoelectric transducer is studied by means of numerical simulations. The governing equations are formulated in a variational framework that, introducing Lagrangian and Hamiltonian densities, is used to derive the weak form for the finite-element discretization of the equations and to characterize the device response in terms of frequency-dependent figures of merit or indicators. The effectiveness of the device in focusing microparticles is quantified by two mechanical indicators: the average direction of the pressure gradient and the amount of acoustic energy localized in the microchannel. Furthermore, we derive the relations between the Lagrangian, the Hamiltonian, and three electrical indicators: the resonance Q value, the impedance, and the electric power. The frequency response of the hard-to-measure mechanical indicators is correlated to that of the easy-to-measure electrical indicators, and, by introducing optimality criteria, it is clarified to which extent the latter suffices to identify optimal driving frequencies as the geometric configuration and the material parameters vary. The latter have been varied by considering both Pyrex and aluminium nitroxide top-lid materials.

General information
State: Published
Organisations: Department of Physics, Biophysics and Fluids, Lund University
Authors: Garofalo, F. (Ekstern), Laurell, T. (Ekstern), Bruus, H. (Intern)
Number of pages: 16
Publication date: 2017
Main Research Area: Technical/natural sciences
Phase-space resolved measurement of 2nd harmonic ion cyclotron heating using FIDA tomography at the ASDEX Upgrade tokamak: Paper

Recent upgrades to the FIDA (fast-ion D-alpha) diagnostic at ASDEX Upgrade allow to reconstruct the fast-ion phase space at several radial positions with decent energy and pitch resolution. These new diagnostic capabilities are applied to study the physics of 2nd harmonic ion cyclotron heating, which is a foreseen heating scenario for ITER. In particular, the acceleration of deuterium beam ions above the injection energy by absorption of ion cyclotron waves at the 2nd harmonic is investigated and compared to theoretical predictions by the TORIC-SSFPQL and TORIC-NUBEAM code packages. Furthermore, comparisons to other fast-ion diagnostics (neutron yield and neutral particle analyzers) are discussed.

General information
State: Published
Organisations: Department of Physics, Plasma Physics and Fusion Energy, Max-Planck-Institut fur Plasmaphysik, University of Seville
Authors: Weiland, M. (Ekstern), Bilato, R. (Ekstern), Geiger, B. (Ekstern), Schneider, P. A. (Ekstern), Tardini, G. (Ekstern), Garcia-Muñoz, M. (Ekstern), Ryter, F. (Ekstern), Salewski, M. (Intern), Zohm, H. (Ekstern)
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Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.51 SNIP 1.62 CiteScore 1.88
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.907 SNIP 1.667 CiteScore 2.2
Web of Science (2014): Indexed yes
Phloem unloading in Arabidopsis roots is convective and regulated by the phloem-pole pericycle

In plants, a complex mixture of solutes and macromolecules is transported by the phloem. Here, we examined how solutes and macromolecules are separated when they exit the phloem during the unloading process. We used a combination of approaches (non-invasive imaging, 3D-electron microscopy, and mathematical modelling) to show that phloem unloading of solutes in Arabidopsis roots occurs through plasmodesmata by a combination of mass flow and diffusion (convective phloem unloading). During unloading, solutes and proteins are diverted into the phloem-pole pericycle, a tissue connected to the protophloem by a unique class of 'funnel plasmodesmata'. While solutes are unloaded without restriction, large proteins are released through funnel plasmodesmata in discrete pulses, a phenomenon we refer to as 'batch unloading'. Unlike solutes, these proteins remain restricted to the phloem-pole pericycle. Our data demonstrate a major role for the phloem-pole pericycle in regulating phloem unloading in roots.
Phonon limited electronic transport in Pb

We present a fully ab initio based scheme to compute electronic transport properties, i.e. the electrical conductivity $\sigma$ and thermopower $S$, in the presence of electron-phonon interaction. We explicitly investigate the $k$-dependent structure of the Eliashberg spectral function, the coupling strength, the linewidth and the relaxation time $\tau$. We obtain a state-dependent $\tau$ and show its necessity to reproduce the increased thermopower for temperatures below the Debye temperature, without accounting for the phonon-drag effect. Despite the detailed investigations of various $k$- and $q$-dependencies, the presented scheme can be easily applied to more complicated systems.
Photocatalysis: HI-time for perovskites

Organolead halide perovskite solar absorbers demonstrate high photovoltaic efficiencies but they are notorious for their intolerance to water. Now, methylammonium lead iodide perovskites are used to harvest solar energy — in water — via photocatalytic generation of hydrogen from solutions of hydriodic acid.

Photothermal Transport of DNA in Entropy-Landscape Plasmonic Waveguides

The ability to handle single, free molecules in lab-on-a-chip systems is key to the development of advanced biotechnologies. Entropic confinement offers passive control of polymers in nanofluidic systems by locally asserting a molecule's number of available conformation states through structured landscapes. Separately, a range of plasmonic configurations have demonstrated active manipulation of nano-objects by harnessing concentrated electric fields. The integration of these two independent techniques promises a range of sophisticated and complementary functions to handle, for example, DNA, but numerous difficulties, in particular, conflicting requirements of channel size, have prevented progress. Here, we show that metallic V-groove waveguides, embedded in fluidic nanoslits, form entropic potentials that trap and guide DNA molecules over well-defined routes while simultaneously promoting photothermal transport of DNA through the losses of plasmonic modes. The propulsive forces, assisted by in-coupling to propagating channel plasmon polaritons, extend along the V-grooves with a directed motion up to \(0.5 \, \mu m \cdot mW^{-1}\) away from the input beam and \(\lambda\)-DNA velocities reaching \(0.2 \, \mu m \cdot s^{-1} \cdot mW^{-1}\). The entropic trapping enables the V-grooves to be flexibly loaded and unloaded with DNA by variation of transverse fluid flow, a process that is selective to biopolymers versus fixed-shape objects and also allows the technique to address the challenges of nanoscale interaction volumes. Our self-aligning, light-driven actuator provides a convenient platform to filter, route, and manipulate individual molecules and may be realized wholly by wafer-scale fabrication suitable for parallelized investigation.
Photovoltaic subretinal implants for blind patients

General information
State: Published
Organisations: Department of Micro- and Nanotechnology, Silicon Microtechnology, Experimental Surface and Nanomaterials Physics, Aarhus University Hospital, Aarhus University
Authors: Davidsen, R. S. (Intern), Bek, T. (Forskerdatabase), Keller, S. S. (Intern), Hansen, O. (Intern)
Number of pages: 1
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Polyol Synthesis of Cobalt–Copper Alloy Catalysts for Higher Alcohol Synthesis from Syngas
Novel catalysts for the selective production of higher alcohols from syngas could offer improved pathways towards synthetic fuels and chemicals. Cobalt–copper alloy catalysts have shown promising results for this reaction. To improve control over particle properties, a liquid phase nanoparticle synthesis based on the polyol method was selected to synthesize Co2.5Cu particles, which were then supported onto a variety of metal oxide supports (Al2O3, SiO2, TiO2, ZrO2). The catalysts were characterized by transmission electron microscopy, X-ray diffraction, and X-ray photoelectron spectroscopy before and after catalytic testing in a flow reactor at 250 °C and 40 bar. The results show alloyed phases were obtained using the polyol method, resulting in selectivity towards higher alcohols, as high as 11.3% when supported on alumina. Segregation of cobalt and the formation of cobalt carbide were observed in the catalysts after catalytic testing, which may limit performance compared to the desired alloy phase.

General information
State: Published
Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics, Stanford University, Universidade Federal do Rio de Janeiro
Authors: Mendes, L. V. (Ekstern), Snider, J. L. (Ekstern), Fleischman, S. D. (Ekstern), Kibsgaard, J. (Intern), McEnaney, J. M. (Ekstern), Jaramillo, T. F. (Ekstern), Aranda, D. A. (Ekstern)
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Scopus rating (2017): SNIP 0.729 SJR 0.73 CiteScore 2.43
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.39 SJR 0.755 SNIP 0.786
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Scopus rating (2015): SJR 0.748 SNIP 0.749 CiteScore 2.27
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BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.89 SNIP 0.928 CiteScore 2.56
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Powder embossing method for selective loading of polymeric microcontainers with drug formulation

The present study introduces powder embossing as a novel method to enhance loading of polymeric microcontainers with drug. With current loading approaches, it is not possible to handle pure powder drug in a scalable, homogenous and reproducible manner. In this work, we demonstrate simultaneous loading of 625 microcontainers with powder formulation. This is achieved in a single step by aligning a shadow mask prepared by micro-milling to an array of microcontainers in order to limit drug deposition to the container cavities with diameters of 220 μm. A pressure of 8.9 MPa is applied by a bonding press and thereby the desired powder is embossed into the container cavities. Powder in the form of pure drug, lipid-based microparticles, and pure polymer was successfully loaded with minimal residues in between the microcontainers and with 100% loaded cavities demonstrating the versatility of the method. The current work is thus contributing to the loading of powder formulations into microscale drug delivery systems such as microcontainers in a facile and reproducible manner.
Scopus rating (2004): SJR 1 SNIP 1.1
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 0.812 SNIP 0.956
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 0.712 SNIP 0.711
Scopus rating (2001): SJR 0.558 SNIP 0.645
Scopus rating (2000): SJR 0.502 SNIP 0.568
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 0.595 SNIP 0.555
Original language: English
Microcontainers, Shadow mask, Micro-milling, Drug delivery systems, Microtomography, Oral drug delivery
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Projects:
Powder embossing method for selective loading of polymeric microcontainers with drug formulation
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Publication: Research - peer-review › Journal article – Annual report year: 2017

Precision of Micro Hall Effect Measurements in Scribe Line Test Pads of B-doped SiGe

General information
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Relations
Activities:
International Conference on Frontiers of Characterization and Metrology for Nanoelectronics 2017
Publication: Research - peer-review › Poster – Annual report year: 2017

Preface: Focus issue to honour Hans L Pécselli on his 70th birthday

General information
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Organisations: Department of Physics, Plasma Physics and Fusion Energy, Umeå University, Linköping University
Authors: Brodin, G. (Ekstern), Stenflo, L. (Ekstern), Rasmussen, J. J. (Intern)
Number of pages: 4
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Main Research Area: Technical/natural sciences

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BFI (2017): BFI-level 1
Probing the Gas-Phase Dynamics of Graphene Chemical Vapour Deposition using *in-situ* UV Absorption Spectroscopy

The processes governing multilayer nucleation in the chemical vapour deposition (CVD) of graphene are important for obtaining high-quality monolayer sheets, but remain poorly understood. Here we show that higher-order carbon species in the gas-phase play a major role in multilayer nucleation, through the use of *in-situ* ultraviolet (UV) absorption spectroscopy. These species are the volatilized products of reactions between hydrogen and carbon contaminants that have backstreamed into the reaction chamber from downstream system components. Consequently, we observe a dramatic suppression of multilayer nucleation when backstreaming is suppressed. These results point to an important and previously undescribed mechanism for multilayer nucleation, wherein higher-order gas-phase carbon species play an integral role. Our work highlights the importance of gas-phase dynamics in understanding the overall mechanism of graphene growth.
Excitons and plasmons are the two most fundamental types of collective electronic excitations occurring in solids. Traditionally, they have been studied separately using bulk techniques that probe their average energetic structure over large spatial regions. However, as the dimensions of materials and devices continue to shrink, it becomes crucial to understand how these excitations depend on local variations in the crystal- and chemical structure on the atomic scale. Here we use monochromated low-loss scanning-transmission-electron-microscopy electron-energy-loss (LL-STEM-EEL) spectroscopy, providing the best simultaneous energy and spatial resolution achieved to-date to unravel the full set of electronic excitations in few-layer MoS$_2$ nanosheets over a wide energy range. Using first-principles many-body calculations we confirm the excitonic nature of the peaks at ~2eV and ~3eV in the experimental EEL spectrum and the plasmonic nature of higher energy-loss peaks. We also rationalise the non-trivial dependence of the EEL spectrum on beam and sample geometry such as the number of atomic layers and distance to steps and edges. Moreover, we show that the excitonic features are dominated by the long wavelength ($q=0$) components of the probing field, while the plasmonic features are sensitive to a much broader range of $q$-vectors, indicating a qualitative difference in the spatial character of the two types of collective excitations. Our work provides a template protocol for mapping the local nature of electronic excitations that open new possibilities for studying photo-absorption and energy transfer processes on a nanometer scale.
Programmable optical waveform reshaping on a picosecond timescale

We experimentally demonstrate the temporal reshaping of optical waveforms in the telecom wavelength band using the principle of quantum frequency conversion. The reshaped optical pulses do not undergo any wavelength translation. The interaction takes place in a nonlinear chi(2) waveguide using an appropriately designed pump pulse programmed via an optical waveform generator. We show the reshaping of a single-peak pulse into a double-peak pulse and vice versa. We also show that exponentially decaying pulses can be reshaped into a near Gaussian shape, and vice versa, which is a useful functionality for quantum communications. (C) 2017 Optical Society of America
Publisher Correction: Invisible Trojan-horse attack
A correction to this article has been published and is linked from the HTML version of this paper. The error has been fixed in the paper.

General information
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Organisations: Department of Physics, Quantum Physics and Information Technology, University of Waterloo
Authors: Sajeev, S. (Ekstern), Minshull, C. (Ekstern), Jain, N. (Intern), Makarov, V. (Ekstern)
Number of pages: 1
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Main Research Area: Technical/natural sciences

Publication information
Journal: Scientific Reports
Volume: 7
Issue number: 1
ISSN (Print): 2045-2322
Pulsed Laser Deposition of YBa$_2$Cu$_3$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 YBa$_2$Cu$_3$O$_x$ 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 YBa$_2$Cu$_3$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.
Element composition transfer, Elements segregation, Pulsed laser deposition, Thin film structure, YBa2Cu3Ox
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
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Main Research Area: Technical/natural sciences
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Pulsed laser deposition (PLD) of the CZTS absorber for thin solar cells with up to 5.2-%-efficiency

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Organisations: Department of Photonics Engineering, Department of Physics, Experimental Surface and Nanomaterials Physics, Silicon Microtechnology, DTU Danchip, Photovoltaic Materials and Systems, Department of Energy Conversion and Storage, Electrofunctional materials, Department of Micro- and Nanotechnology, University of New South Wales
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Electronic versions:
MRS_2017_poster_JS_2.pdf

Pump-Enhanced Continuous-Wave Magnetometry Using Nitrogen-Vacancy Ensembles
Ensembles of nitrogen-vacancy centers in diamond are a highly promising platform for high-sensitivity magnetometry, whose efficacy is often based on inefficiently generating and monitoring magnetic-field dependent infrared fluorescence. Here we report on an increased sensing efficiency with the use of a 532-nm resonant confocal cavity and a microwave resonator antenna for measuring the local magnetic noise density using the intrinsic nitrogen-vacancy concentration of a chemical-vapor deposited single-crystal diamond. We measure near-shot-noise-limited magnetic noise floor of 200 pT/√Hz spanning a bandwidth up to 159 Hz, and an extracted sensitivity of approximately 3 nT/√Hz, with further enhancement limited by the noise floor of the lock-in amplifier and the laser damage threshold of the optical components. Exploration of the microwave and optical pump-rate parameter space demonstrates a linewidth-narrowing regime reached by virtue of the optical cavity, allowing an enhanced sensitivity to be achieved, despite an unoptimized collection efficiency of about 0.2 ppb.

General information
State: Published
Organisations: Department of Physics, Quantum Physics and Information Technology
Authors: Ahmadi, S. (Intern), El-Ella, H. A. R. (Intern), Hansen, J. O. B. (Ekstern), Huck, A. (Intern), Andersen, U. L. (Intern)
Number of pages: 10
Quantification of liquid products from the electroreduction of CO$_2$ and CO using static headspace-gas chromatography and nuclear magnetic resonance spectroscopy

Static headspace-gas chromatography (HS-GC) useful for ex-situ liquid product analysis. Could complement high-performance liquid chromatography and NMR spectroscopy. Particularly high sensitivity towards compounds with high vapor pressure. Detection limits below 0.5μM were shown for acetaldehyde and propionaldehyde. Cannot detect protonated compounds such as formate and acetate.
As described in the previous chapters, optical tweezers have become a tool of precision for in vitro single-molecule investigations, where the single molecule of interest most often is studied in purified form in an experimental assay with a well-controlled fluidic environment. A well-controlled fluidic environment implies that the physical properties of the liquid, most notably the viscosity, are known and the fluidic environment can, for calibrational purposes, be treated as a simple...
In vivo, however, optical tweezers have primarily been used as a tool of manipulation and not so often for precise quantitative force measurements, due to the unknown value of the spring constant of the optical trap formed within the cell’s viscoelastic cytoplasm. Here, we describe a method for utilizing optical tweezers for quantitative in vivo force measurements. The experimental protocol and the protocol for data analysis rely on two types of experiments, passive observation of the thermal motion of a trapped object inside a living cell, followed by observations of the response of the trapped object when subject to controlled oscillations of the optical trap. One advantage of this calibration method is that the size and refractive properties of the trapped object and the viscoelastic properties of its environment need not be known. We explain the protocol and demonstrate its use with experiments of trapped granules inside live S. pombe cells.

Quantitative Image Simulation and Analysis of Nanoparticles

Materials science increasingly relies on powerful microscopes to study the relationship between a material property and its underlying structure. Understanding this relationship is critical for catalysis, due to the importance of structure at the nanoscale. High-Resolution Transmission Electron Microscopy (HRTEM) has become a routine analysis tool for structural characterization at atomic resolution, and with the recent development of in-situ TEMs, it is now possible to study catalytic nanoparticles under reaction conditions. However, the connection between an experimental image, and the underlying physical phenomena or structure is not always straightforward. The aim of this thesis is to use image simulation to better understand observations from HRTEM images. Surface strain is known to be important for the performance of nanoparticles. Using simulation, we estimate the precision and accuracy of strain measurements from TEM images, and investigate the stability of these measurements to microscope parameters. This is followed by our efforts toward simulating metal nanoparticles on a metal-oxide support using the Charge Optimized Many Body (COMB) interatomic potential. The simulated interface structures are used as input for image simulations, to understand how support-induced strain influences a HRTEM image.

This thesis also introduces two novel analysis tools for atomic-resolution images. The first tool is an automatic method for calculating strain from HRTEM images with several advantages over previous methods. The second tool, is a neural network based algorithm for recognition of the local structure in images. The neural network was trained entirely from image simulations, but is capable of making correct predictions on experimental images.
Qudi: a modular python suite for experiment control and data processing
Qudi is a general, modular, multi-operating system suite written in Python 3 for controlling laboratory experiments. It provides a structured environment by separating functionality into hardware abstraction, experiment logic and user interface layers. The core feature set comprises a graphical user interface, live data visualization, distributed execution over networks, rapid prototyping via Jupyter notebooks, configuration management, and data recording. Currently, the included modules are focused on confocal microscopy, quantum optics and quantum information experiments, but an expansion into other fields is possible and encouraged. Qudi is available from https://github.com/Ulm-IQO/qudi and is freely useable under the GNU General Public Licence.

RAMI analysis of the ITER LFS CTS system
This paper describes an initial RAMI analysis for the ITER Low Field Side Collective Thomson Scattering system (LFS CTS) based on its preliminary architecture at system design level. The benefits and challenges involved in this analysis since an early phase of the design are discussed together with the methodology pursued. The Functional Analysis, developed both at system and sub-system level, are the major inputs for the RAMI analysis. A systematic approach has been used, and significant design assumptions have been made due to the lack of knowledge and definition inherent to preliminary design stages. This study includes the Failure Mode, Effects and Criticality Analysis and the Reliability Block Diagram of the system. The results obtained for the system Availability and Reliability are presented and discussed, and criticality charts are developed to highlight the risk levels of the failure modes, regarding to their likelihood and effects on the Availability of the ITER machine. Mitigation actions are proposed to reduce these risk levels in case of impact on the ITER operation.
Reaction mechanism of dimethyl ether carbonylation to methyl acetate over mordenite: a combined DFT/experimental study

The reaction mechanism of dimethyl ether carbonylation to methyl acetate over mordenite was studied theoretically with periodic density functional theory calculations including dispersion forces and experimentally in a fixed bed flow reactor at pressures between 10 and 100 bar, dimethyl ether concentrations in CO between 0.2 and 2.0%, and at a temperature of 438 K. The theoretical study showed that the reaction of CO with surface methyl groups, the rate-limiting step, is faster in the eight-membered side pockets than in the twelve-membered main channel of the zeolite; the subsequent reaction of dimethyl ether with surface acetyl to form methyl acetate was demonstrated to occur with low energy barriers in both the side pockets and in the main channel. The present analysis has thus identified a path, where the entire reaction occurs favourably on a single site within the side pocket, in good agreement with previous experimental studies. The experimental study of the reaction kinetics was consistent with the theoretically derived mechanism and in addition revealed that the methyl acetate product inhibits the reaction - possibly by sterically hindering the attack of CO on the methyl groups in the side pockets.

General information
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Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, Department of Physics, Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry, Haldor Topsoe AS, SLAC National Accelerator Laboratory
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Scopus rating (2015): SJR 1.804 SNIP 1.314 CiteScore 5.46
Web of Science (2015): Indexed yes
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Real-time detection of sub-monolayer desorption phenomena during electrochemical reactions: Instrument development and applications

This thesis presents the development of a novel analysis instrument for performing highly sensitive electrochemistry mass spectrometry (EC-MS) measurements in real-time. The instrument is based on a micofabricated membrane chip which is used to establish a direct loss-free coupling between wet electrochemistry and the vacuum of a mass spectrometer, thereby enabling a high detection probability of volatile analyte species by the mass spectrometer. The instrument exhibits a higher sensitivity than conventional differential electrochemical mass spectrometry (DEMS), while maintaining a fast response time, making it highly suitable for electrochemistry studies.

Incorporating the membrane chip into a stagnant thin-layer electrochemistry cell, 100% collection efficiency is ensured, which makes it possible to utilize the full dynamic range of a standard MS, and thereby analyze desorption phenomena during electrochemical measurements with sub-monolayer sensitivity. The membrane chip furthermore makes it possible to directly control the dissolved gas atmosphere experienced by the working electrode by dosing gases through the membrane. Thereby reactant gases can be introduced, either for steady-state electrocatalytic measurements, or by transiently perturbing the system with single pulses of reactant gas injections.

The capabilities of the instrumentation are demonstrated by studying electrochemical hydrogen evolution (HER), oxygen evolution (OER), CO oxidation and CO stripping on polycrystalline platinum. The latter two are made possible by the transient and steady-state introduction CO reactant gas, respectively, through the membrane. A mass transport model is used to describe the analytetransport from the surface of an electrode, through the stagnant thin-layer cell, through the membrane chip and into the mass spectrometer. By applying this model to HER, OER, CO oxidation and CO stripping experiments, it is demonstrated possible to match anticipated mass spectrometer signals based on current measurements on the electrode, to the actual measured mass spectrometer signal. This mapping function thereby directly couples mass spectrometer data with faradaic currents on the electrode surface.

The EC-MS instrumentation presented herein is utilized to discover a new electrocatalytic phenomenon during electrochemical CO reduction: By exposing a copper catalyst to dioxygen prior to constant-potential electrolysis, a new reaction pathway towards methane production is temporarily established. The phenomenon is shown only to affect the formation of methane, leaving ethylene and hydrogen formation unaffected. Using density functional theory (DFT) it is demonstrated that adsorbed oxygen on surface sites adjacent to undercoordinated kink sites destabilizes the binding energy of CO, while stabilizing the binding energy of CHO due to a geometric tilting effect. This causes the initial protonation towards methane, which is otherwise known to be rate-limiting on kink sites, to become energetically favorable. The phenomenon is short-lived, as the adsorbed oxygen reduces away within ~1 s during which only a few turnovers of methane occurs.

Furthermore, a preliminary EC-MS study is presented, which reveals a new desorption phenomenon on polycrystalline copper: By initially priming a copper electrode at cathodic potentials close to hydrogen evolution potentials, the desorption of ~ 50 pmol of gaseous hydrogen, corresponding to ~ 10% of a monolayer, is measured when scanning to potential anodic of the reversible hydrogen potential (RHE). The phenomenon is proven to be electrochemically triggered, unrelated to copper oxidation and invariant to pH on the RHE scale. The amount of desorbed hydrogen is likewise proven to be unaffected by priming conditions and potential scan rates. By variation of the upper and lower potential limits the ad- and desorption potentials for hydrogen on copper are measured to be -0.125 and +0.05 V vs RHE, respectively. The proposed mechanism is that hydrogen adsorbs to the surface at cathodic potentials prior to HER, and remain surface bound until it becomes energetically favorable to adsorb OH at more cathodic potentials, at which hydrogen is expelled through a surface replacement reaction. As only ~10% of a monolayer, is observed, the hydrogen is believed only to remain adsorbed on stronger binding step sites. The proposed mechanism is not yet verified with any theoretical predictions. The presented electrochemical studies exemplifies some of the unique capabilities enabled by the presented EC-MS instrumentation. The potential for future application of the technique could be wide-spread and enable unique insight into electrochemical reaction mechanism through careful study of sub-monolayer desorption phenomena similar to the ones presented herein.

General information
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Real-time detection of sub-monolayer desorption phenomena during electrochemical reactions: Instrument development and applications

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Recent development of collective Thomson scattering for magnetically confined fusion plasmas

Here we review recent experimental developments within the field of collective Thomson scattering with a focus on the progress made on the devices TEXTOR and ASDEX Upgrade. We discuss recently discovered possibilities and limitations of the diagnostic technique. Diagnostic applications with respect to ion measurements are demonstrated. Examples include measurements of the ion temperature, energetic ion distribution function, and the ion composition.

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Web of Science (2010): Indexed yes
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Recent H majority inverted radio frequency heating scheme experiments in JET-ILW

Inverted 3He and D ion cyclotron minority heating scenarios were recently tested in JET-ILW. They confirm the good heating efficiency at low concentrations of ~3%. The 3He minority heating scheme is only modestly affected by the change from a carbon (JET-C) to a Beryllium (JET-ILW) wall but unlike what was the case in JET-C, the intrinsic Be ions D-like particles in terms of charge-over-mass ratio do not prevent the D (or 4He) minority regime from being exploited. Direct and indirect evidence of the existence of fast particle subpopulations was found in both cases.

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Recent progress towards a quantitative description of filamentary SOL transport

A summary of recent results on filamentary transport, mostly obtained with the ASDEX-Upgrade tokamak (AUG), is presented and discussed in an attempt to produce a coherent picture of scrape-off layer (SOL) filamentary transport. A clear correlation is found between L-mode density shoulder formation in the outer midplane and a transition between the sheath-limited and the inertial filamentary regimes. Divertor collisionality is found to be the parameter triggering the transition. A clear reduction of the ion temperature takes place in the far SOL after the transition, both for the background and the filaments. This coincides with a strong variation of the ion temperature distribution, which deviates from Gaussianity and becomes dominated by a strong peak below 5 eV. The filament transition mechanism triggered by a critical value of collisionality seems to be generally applicable to inter-ELM H-mode plasmas, although a secondary threshold related to deuterium fueling is observed. EMC3-EIRENE simulations of neutral dynamics show that an ionization front near the main chamber wall is formed after the shoulder formation. Finally, a clear increase of SOL opacity to neutrals is observed, associated with the shoulder formation. A common SOL transport framework is proposed to account for all these results, and their potential implications for future generation devices are discussed.

General information
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Web of Science (2014): Indexed yes
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Reconsidering Water Electrolysis: Producing Hydrogen at Cathodes Together with Selective Oxidation of n-Butylamine at Anodes

Electrocatalysis for the oxygen evolution reaction (OER) is of great interest for improving the effectiveness of water splitting devices. Decreasing the anodic overpotential and simultaneously changing the anodic reaction selectively to produce valuable chemicals instead of \( \text{O}_2 \) would be a major improvement of the overall cost efficiency. Some amines, when present in aqueous electrolytes, were recently shown to change the selectivity of the anodic process to generate \( \text{H}_2 \) \( \text{O}_2 \) rather than \( \text{O}_2 \) on \( \text{MnO}_x \) at pH 10. This results in unusually high apparent “anodic activities”. In this work, industrially relevant OER catalysts, oxyhydroxides of cobalt (\( \text{CoO}_x \)), nickel–iron (\( \text{NiFeO}_x \)), and nickel (\( \text{NiO}_x \)) all show more pronounced effects. Moreover, as anodes they also selectively catalyzed the production of n-butyronitrile from n-butylamine at higher pH as an easily retrievable valuable product. The pH dependence of the activity was investigated at pH values closer those at which alkaline electrolyzers operate. The highest activities were observed for \( \text{NiO}_x \) thin-film electrodes at pH 12 in the presence of 0.4 m n-butylammonium sulfate, without poisoning the active sites of Pt electrocatalysts at the hydrogen evolution electrode. \(^1\)H NMR spectroscopy showed that n-butylamine is selectively oxidized to n-butyronitrile, an organic chemical with numerous applications. However, measurements using rotating ring-disk electrodes indicated that some \( \text{H}_2\text{O}_2 \) is also generated at the surface of the oxide anodes.
Roadmap for optofluidics

Optofluidics, nominally the research area where optics and fluidics merge, is a relatively new research field and it is only in the last decade that there has been a large increase in the number of optofluidic applications, as well as in the number of research groups, devoted to the topic. Nowadays optofluidics applications include, without being limited to, lab-on-a-chip devices, fluid-based and controlled lenses, optical sensors for fluids and for suspended particles, biosensors, imaging tools, etc. The long list of potential optofluidics applications, which have been recently demonstrated, suggests that optofluidic technologies will become more and more common in everyday life in the future, causing a significant impact on
many aspects of our society. A characteristic of this research field, deriving from both its interdisciplinary origin and applications, is that in order to develop suitable solutions a combination of a deep knowledge in different fields, ranging from materials science to photonics, from microfluidics to molecular biology and biophysics, is often required. As a direct consequence, also being able to understand the long-term evolution of optofluidics research is not easy. In this article, we report several expert contributions on different topics so as to provide guidance for young scientists. At the same time, we hope that this document will also prove useful for funding institutions and stakeholders to better understand the perspectives and opportunities offered by this research field.
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.
Roughness in flatland

Energy-favoured grain rotation in nanocrystalline metals is shown to cause surface roughness at the atomic scale, providing fundamental insight for grain boundary engineering in materials design.

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Scene reassembly after multimodal digitization and pipeline evaluation using photorealistic rendering

Transparent objects require acquisition modalities that are very different from the ones used for objects with more diffuse reflectance properties. Digitizing a scene where objects must be acquired with different modalities requires scene
reassembly after reconstruction of the object surfaces. This reassembly of a scene that was picked apart for scanning seems unexplored. We contribute with a multimodal digitization pipeline for scenes that require this step of reassembly. Our pipeline includes measurement of bidirectional reflectance distribution functions and high dynamic range imaging of the lighting environment. This enables pixelwise comparison of photographs of the real scene with renderings of the digital version of the scene. Such quantitative evaluation is useful for verifying acquired material appearance and reconstructed surface geometry, which is an important aspect of digital content creation. It is also useful for identifying and improving issues in the different steps of the pipeline. In this work, we use it to improve reconstruction, apply analysis by synthesis to estimate optical properties, and to develop our method for scene reassembly.

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Scopus rating (2012): SJR 1.042 SNIP 1.468 CiteScore 1.79
ISI indexed (2012): ISI indexed no
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.055 SNIP 1.744 CiteScore 1.92
ISI indexed (2011): ISI indexed no
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.079 SNIP 1.603
Web of Science (2010): Indexed yes
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Scopus rating (2009): SJR 1.2 SNIP 1.678
Web of Science (2009): Indexed yes
Simple vertex correction improves GW band energies of bulk and two-dimensional crystals

The GW self-energy method has long been recognized as the gold standard for quasiparticle (QP) calculations of solids in spite of the fact that the neglect of vertex corrections and the use of a density-functional theory starting point lack rigorous justification. In this work we remedy this situation by including a simple vertex correction that is consistent with a local-density approximation starting point. We analyze the effect of the self-energy by splitting it into short-range and long-range terms which are shown to govern, respectively, the center and size of the band gap. The vertex mainly improves the short-range correlations and therefore has a small effect on the band gap, while it shifts the band gap center up in energy by around 0.5 eV, in good agreement with experiments. Our analysis also explains how the relative importance of short- and long-range interactions in structures of different dimensionality is reflected in their QP energies. Inclusion of the vertex comes at practically no extra computational cost and even improves the basis set convergence compared to GW. Taken together, the method provides an efficient and rigorous improvement over the GW approximation.
Simulating and optimizing compound refractive lens-based X-ray microscopes

A comprehensive optical description of compound refractive lenses (CRLs) in condensing and full-field X-ray microscopy applications is presented. The formalism extends ray-transfer matrix analysis by accounting for X-ray attenuation by the lens material. Closed analytical expressions for critical imaging parameters such as numerical aperture, spatial
acceptance (vignetting), chromatic aberration and focal length are provided for both thin- and thick-lens imaging geometries. These expressions show that the numerical aperture will be maximized and chromatic aberration will be minimized at the thick-lens limit. This limit may be satisfied by a range of CRL geometries, suggesting alternative approaches to improving the resolution and efficiency of CRLs and X-ray microscopes.
SiO₂ Glass Density to Lower-Mantle Pressures

The convection or settling of matter in the deep Earth's interior is mostly constrained by density variations between the different reservoirs. Knowledge of the density contrast between solid and molten silicates is thus of prime importance to understand and model the dynamic behavior of the past and present Earth. SiO₂ is the main constituent of Earth's mantle and is the reference model system for the behavior of silicate melts at high pressure. Here, we apply our recently developed x-ray absorption technique to the density of SiO₂ glass up to 110 GPa, doubling the pressure range for such measurements. Our density data validate recent molecular dynamics simulations and are in good agreement with previous experimental studies conducted at lower pressure. Silica glass rapidly densifies up to 40 GPa, but the density trend then flattens to become asymptotic to the density of SiO₂ minerals above 60 GPa. The density data present two discontinuities at similar to 17 and similar to 60 GPa that can be related to a silicon coordination increase from 4 to a mixed 5/6 coordination and from 5/6 to sixfold, respectively. SiO₂ glass becomes denser than MgSiO₃ glass at similar to 40 GPa, and its density becomes identical to that of MgSiO₃ glass above 80 GPa. Our results on SiO₂ glass may suggest that a variation of SiO₂ content in a basaltic or pyroilitic melt with pressure has at most a minor effect on the final melt density, and iron partitioning between the melts and residual solids is the predominant factor that controls melt buoyancy in the lowermost mantle.

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Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Universitat Bayreuth, Swiss Federal Laboratories for Materials Science and Technology (Empa), Universite Grenoble Alpes, Sorbonne Universités, European Synchrotron Radiation Facility
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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.

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Scopus rating (2014): SJR 0.615 SNIP 0.792 CiteScore 2.05
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Sparse identification of a predator-prey system from simulation data of a convection model

The use of low-dimensional dynamical systems as reduced models for plasma dynamics is useful as solving an initial value problem requires much less computational resources than fluid simulations. We utilize a data-driven modeling approach to identify a reduced model from simulation data of a convection problem. A convection model with a pressure source centered at the inner boundary models the edge dynamics of a magnetically confined plasma. The convection problem undergoes a sequence of bifurcations as the strength of the pressure source increases. The time evolution of the energies of the pressure profile, the turbulent flow, and the zonal flow capture the fundamental dynamic behavior of the full system. By applying the sparse identification of nonlinear dynamics (SINDy) method, we identify a predator-prey type dynamical system that approximates the underlying dynamics of the three energy state variables. A bifurcation analysis of the system reveals consistency between the bifurcation structures, observed for the simulation data, and the identified underlying system.

General information
State: Published
Authors: Dam, M. (Intern), Brøns, M. (Intern), Rasmussen, J. J. (Intern), Naulin, V. (Intern), Hesthaven, J. S. (Ekstern)
Number of pages: 10
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Main Research Area: Technical/natural sciences

Publication information
Spectral correction algorithm for multispectral CdTe x-ray detectors

Compared to the dual energy scintillator detectors widely used today, pixelated multispectral X-ray detectors show the potential to improve material identification in various radiography and tomography applications used for industrial and security purposes. However, detector effects, such as charge sharing and photon pileup, distort the measured spectra in high flux pixelated multispectral detectors. These effects significantly reduce the detectors’ capabilities to be used for material identification, which requires accurate spectral measurements. We have developed a semi analytical computational algorithm for multispectral CdTe X-ray detectors which corrects the measured spectra for severe spectral distortions caused by the detector. The algorithm is developed for the Multix ME100 CdTe X-ray detector, but could potentially be adapted for any pixelated multispectral CdTe detector. The calibration of the algorithm is based on simple attenuation measurements of commercially available materials using standard laboratory sources, making the algorithm applicable in any X-ray setup. The validation of the algorithm has been done using experimental data acquired with both standard lab equipment and synchrotron radiation. The experiments show that the algorithm is fast, reliable even at X-ray flux up to 5 MPk/s/mm², and greatly improves the accuracy of the measured X-ray spectra, making the algorithm very useful for both security and industrial applications where multispectral detectors are used.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, University of Copenhagen, European XFEL
Authors: Christensen, E. D. (Ekstern), Kehres, J. (Intern), Gu, Y. (Intern), Feidenhans'l, R. (Ekstern), Olsen, U. L. (Intern)
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Multispectral CdTe detectors, Compensation of spectral distortions, Photon-counting, Multix ME100, Pulse pileup correction, Charge sharing correction

Spin-dependent electron-phonon coupling in the valence band of single-layer WS₂

The absence of inversion symmetry leads to a strong spin-orbit splitting of the upper valence band of semiconducting single-layer transition-metal dichalcogenides such as MoS₂ or WS₂. This permits a direct comparison of the electron-phonon coupling strength in states that only differ by their spin. Here, the electron-phonon coupling in the valence band maximum of single-layer WS₂ is studied by first-principles calculations and angle-resolved photoemission. The coupling strength is found to be drastically different for the two spin-split branches, with calculated values of λ_K=0.0021 and 0.40 for the upper and lower spin-split valence band of the freestanding layer, respectively. This difference is somewhat reduced when including scattering processes involving the Au(111) substrate present in the experiment but it remains significant, in good agreement with the experimental results.

General information
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Organisations: Department of Physics, Theoretical Atomic-scale Physics, Aarhus University, University of Trieste, Elettra Sincrotrone Trieste, Consiglio Nazionale delle Ricerche
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Web of Science (2016): Indexed yes
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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
Spin excitations and quantum criticality in the quasi-one-dimensional Ising-like ferromagnet CoCl₂·2D₂O in a transverse field

We present experimental evidence for a quantum phase transition in the easy-axis $S = \frac{3}{2}$ anisotropic quasi-one-dimensional ferromagnet CoCl₂·2D₂O in a transverse field. Elastic neutron scattering shows that the magnetic order parameter vanishes at a transverse critical field $\mu_0 H_c = 16.05(4)$ T, while inelastic neutron scattering shows that the gap in the magnetic excitation spectrum vanishes at the same field value, and reopens for $H > H_c$. The field dependence of the order parameter and the gap are well described by critical exponents $\beta = 0.45 \pm 0.09$ and $z \nu$ close to $1/2$, implying that the quantum phase transition in CoCl₂·2D₂O differs significantly from the textbook version of a $S = 1/2$ Ising chain in a transverse field. We attribute the difference to weak but finite three-dimensionality of the magnetic interactions.
Spin orientation in solid solution hematite-ilmenite

The spin orientation in synthetic hematite-ilmenite samples and in a sample of natural hematite was studied from room temperature to above the antiferromagnetic-paramagnetic phase transition (the Néel temperature; TN = 600–950 K) by neutron powder diffraction and at room temperature by Mössbauer spectroscopy. The usually assumed magnetic structure of hematite within this temperature range is antiferromagnetic with the spins confined to the basal plane of the hexagonal structure; however, an out-of-plane spin component is allowed by the symmetry of the system and has been observed in recent studies of synthetic hematite samples. We find the spins in the antiferromagnetic sublattices to be rotated out of the basal plane by an angle between 11(2)° and 22.7(5)° in both synthetic hematite-ilmenite samples and in the natural hematite sample. The spin angle remains tilted out of the basal plane in the entire temperature range below the Néel temperature and does not depend systematically on Ti-content. The results indicate that the out-of-plane spin component is an intrinsic feature of hematite itself, with an origin not yet fully understood, but consistent with group theory. This represents a major shift in understanding of one of the two main mineral systems responsible for rock magnetism.

General information

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Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, University of Copenhagen, Norwegian University of Science and Technology, Geological Survey of Norway, National Institute of Standards and Technology, University of Cambridge, Institut Max von Laue-Paul Langevin
Authors: Brok, E. (Intern), Frandsen, C. (Intern), Lefmann, K. (Ekstern), McEnroe, S. A. (Ekstern), Robinson, P. (Ekstern), Burton, B. P. (Ekstern), Hansen, T. C. (Ekstern), Harrison, R. (Ekstern)
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Scopus rating (2016): SJR 0.962 SNIP 0.975 CiteScore 1.88
Web of Science (2016): Indexed yes
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Scopus rating (2015): SJR 1.156 SNIP 1.021 CiteScore 2.01
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Scopus rating (2014): SJR 1.225 SNIP 1.138 CiteScore 1.94
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ISI indexed (2013): ISI indexed yes
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Scopus rating (2012): SJR 1.44 SNIP 1.323 CiteScore 2.19
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.679 SNIP 1.306 CiteScore 2.17
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.591 SNIP 1.232
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.533 SNIP 1.192
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.818 SNIP 1.417
Scopus rating (2007): SJR 1.891 SNIP 1.316
Scopus rating (2006): SJR 1.8 SNIP 1.365
Scopus rating (2005): SJR 1.565 SNIP 1.274
Scopus rating (2004): SJR 1.616 SNIP 1.305
Scopus rating (2003): SJR 1.446 SNIP 1.248
Scopus rating (2002): SJR 1.802 SNIP 1.459
Scopus rating (2001): SJR 1.859 SNIP 1.216
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 1.722 SNIP 1.644
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Spray-coated Cu2ZnSnS4 thin films for large-scale photovoltaic applications

The kesterite material, Cu2ZnSnS4 (CZTS), has in the preceding ten years been investigated and developed as a new Earth-abundant material for solar cells. The interest in this inorganic semiconductor originates in its optimal energy band gap of approx. 1.5 eV, high absorption coefficient, and the high material abundance and low toxicity of all elements included. The current challenges are related to unavoidable antisite disordering stemming from the chemical similarity of the cations, which causes bulk defects and lowers the open-circuit voltage detrimentally. This, however, did not restrict the "cousin"-material, CulnGaSe2 (CIGS), which is currently one of the main thin-film photovoltaic (PV) technologies on the market. In this work, CZTS thin films have been fabricated by solution-processing, which allows relatively fast and inexpensive deposition when compared to vacuum-processed films. The nanoparticles are synthesized by the hot-injection method by mixing targeted ratios of metal salts with sulfur in diethylene glycol, resulting in a phase-pure CZTS material [1]. Inks are formulated by dispersing the particles in ethanol and water using a suitable dispersing agent. The solvents used allow that alkali metal chloride salts can also be dissolved in controllable amounts, which we have found enhances grain growth in the films during the subsequent annealing step. A Sono-tek spray-coating system with ultrasonic atomization is used. We investigate the effect of ink concentration, and spray-coating conditions, including spray power, flow rate from syringe pump, and time between consecutive spray layers. The films are annealed in a tube furnace, and to avoid decomposing the material into secondary phases, a graphite box is used to enable an overpressure of sulfur and tin-sulfide. The annealed, spray-coated films are characterized by scanning electron microscopy (SEM), optical microscopy, and Dektak profilometry.

Stability of a Bifunctional Cu-Based Core@Zeolite Shell Catalyst for Dimethyl Ether Synthesis Under Redox Conditions Studied by Environmental Transmission Electron Microscopy and In Situ X-Ray Ptychography

When using bifunctional core@shell catalysts, the stability of both the shell and core-shell interface is crucial for catalytic applications. In the present study, we elucidate the stability of a CuO/ZnO/Al2O3@ZSM-5 core@shell material, used for one-stage synthesis of dimethyl ether from synthesis gas. The catalyst stability was studied in a hierarchical manner by complementary environmental transmission electron microscopy (ETEM), scanning electron microscopy (SEM) and in situ hard X-ray ptychography in situ. Both reductive activation and reoxidation were applied. The core-shell interface was found to be stable during reducing and oxidizing treatment at 250°C as observed by ETEM and in situ X-ray ptychography. Nevertheless, the crucial core-shell interface required for full bifunctionality appeared to remain stable. This study demonstrates the potential of these correlative in situ microscopy techniques for hierarchically designed catalysts.

General information
State: Published
Organisations: Department of Photonics Engineering, Photovoltaic Materials and Systems, Department of Micro- and Nanotechnology, Silicon Microtechnology, Experimental Surface and Nanomaterials Physics, InMold Biosystems A/S
Authors: Engberg, S. L. J. (Intern), Murthy, S. (Ekstern), Mariño, S. L. (Intern), Hansen, O. (Intern), Kofod, G. (Ekstern), Schou, J. (Intern)
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Organisations: Center for Electron Nanoscopy, Department of Physics, Experimental Surface and Nanomaterials Physics, Karlsruhe Institute of Technology KIT, Friedrich-Alexander University Erlangen-Nuremberg, Deutsches Elektronensynchrotron DESY, Universität Hamburg
Authors: Baier, S. (Ekstern), Damsgaard, C. D. (Intern), Klumpp, M. (Ekstern), Reinhardt, J. (Ekstern), Sheppard, T. (Ekstern), Balogh, Z. I. (Intern), Kasama, T. (Intern), Benzi, F. (Ekstern), Wagner, J. B. (Intern), Schwieger, W. (Ekstern), Schroer, C. G. (Ekstern), Grunwaldt, J. (Ekstern)
Staging superstructures in high-Tc Sr/O co-doped La$_{2-x}$Sr$_x$CuO$_{4+y}$

We present high-energy x-ray diffraction studies on the structural phases of an optimal high-Tc superconductor La$_{2-x}$Sr$_x$CuO$_{4+y}$ tailored by co-hole-doping. This is specifically done by varying the content of two very different chemical species, Sr and O, respectively, in order to study the influence of each. A superstructure known as staging is observed in all samples, with the staging number n increasing for higher Sr dopings x. We find that the staging phases emerge abruptly with temperature, and can be described as a second-order phase transition with transition temperatures slightly depending on the Sr doping. The Sr appears to correlate the interstitial oxygen in a way that stabilizes the reproducibility of the staging phase both in terms of staging period and volume fraction in a specific sample. The structural details as investigated in this paper appear to have no direct bearing on the electronic phase separation previously observed in the same samples. This provides evidence that the electronic phase separation is determined by the overall hole concentration rather than specific Sr/O content and concomitant structural details.

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Web of Science (2017): Indexed yes
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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
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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 3.236 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
Stochastic derivation and solution of simplified radiative transfer using the Fokker-Planck equation

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, Neutrons and X-rays for Materials Physics, Technical University of Denmark
Authors: Linder-Steinlein, K. (Ekstern), Chen, X. (Ekstern), Karamehmedovic, M. (Intern)
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Main Research Area: Technical/natural sciences
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Kris_Xi_MK_poster.pdf
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Strategies for stable water splitting via protected photoelectrodes
Photoelectrochemical (PEC) solar-fuel conversion is a promising approach to provide clean and storable fuel (e.g., hydrogen and methanol) directly from sunlight, water and CO₂. However, major challenges still have to be overcome before commercialization can be achieved. One of the largest barriers to overcome is to achieve a stable PEC reaction in either strongly basic or acidic electrolytes without degradation of the semiconductor photoelectrodes. In this work, we discuss fundamental aspects of protection strategies for achieving stable solid/liquid interfaces. We then analyse the charge transfer photocathodes. In addition, we review protection layer approaches and their stabilities for a wide variety of experimental photoelectrodes for water reduction. Finally, we discuss key aspects which should be addressed in continued work on realizing stable and practical PEC solar water splitting systems.

General information
State: Published
Strong Plasmon-Phonon Splitting and Hybridization in 2D Materials Revealed through a Self-Energy Approach

We reveal new aspects of the interaction between plasmons and phonons in 2D materials that go beyond a mere shift and increase in plasmon width due to coupling to either intrinsic vibrational modes of the material or phonons in a supporting substrate. More precisely, we predict strong plasmon splitting due to this coupling, resulting in a characteristic avoided crossing scheme. We base our results on a computationally efficient approach consisting in including many-body interactions through the electron self-energy. We specify this formalism for a description of plasmons based upon a tight-binding electron Hamiltonian combined with the random-phase approximation. This approach is valid provided vertex corrections can be neglected, as is the case in conventional plasmon-supporting metals and Dirac-Fermion systems. We illustrate our method by evaluating plasmonic spectra of doped graphene nanotriangles with varied size, where we predict remarkable peak splittings and other radical modifications in the spectra due to plasmon interactions with intrinsic optical phonons. Our method is equally applicable to other 2D materials and provides a simple approach for investigating coupling of plasmons to phonons, excitons, and other excitations in hybrid thin nanostructures.
Structural Analysis Algorithms for Nanomaterials
This thesis presents a reformulation of existing problems in materials science in terms of well-known methods from applied mathematics: graph theory, computational geometry, and mixed integer programming.

The centrosymmetry parameter is reformulated as a graph matching problem, and resolves the inconsistencies in the existing calculation methods as a consequence. By formulating the distance function of lattices as a bipartite graph matching problem, it is shown that the similarity between crystal lattices (root mean square distance, RMSD) can be calculated in polynomial time, which improves upon the existing factorial-time bound. This method is subsequently extended to two-dimensional monolayers.

A method is presented for the identification of ordered crystalline phases in molecular dynamics simulations. A robust classification is obtained by the use of template matching, also formulated as a bipartite matching problem on geometric graphs. This method is adapted for two-dimensional materials, in order that e.g. defect structures in polycrystalline graphene can be studied.

Matrix decompositions are used to develop a geometric lattice matching algorithm, which can exhaustively identify all low-strain interfaces. The stable, low-energy interfaces which are found as a result are intended for use in the design and construction of topological superconductors, which have important applications in quantum computing.

Cluster expansion models are used to find ground-state structures in gold-silver nanoparticles, which are used in a variety of catalysis processes. In addition to this concrete application, theoretical methods are developed for the optimal construction of cluster expansion models, the exact determination of ground states in a large model, and the exhaustive determination of all possible ground states in a small model.

Lastly, a method for nearly-optimal sampling of orientations is presented. Whilst this has many applications in science and engineering, the use-case described here is the indexing of diffraction patterns for experimental materials characterization. Significantly improved sampling is achieved by applying methods from computational geometry.

General information
State: Published
Organisations: Department of Physics, Theoretical Atomic-scale Physics, Neutrons and X-rays for Materials Physics
Authors: Larsen, P. M. (Intern), Schiøtz, J. (Intern), Schmidt, S. (Intern)
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Structural stability of naphthyl end-capped oligothiophenes in organic field-effect transistors measured by grazing-incidence X-ray diffraction in operando
We report on microstructural durability of 5,5′-bis(naphth-2-yl)-2,2′-bithiophene (NaT2) in organic field-effect transistors (OFETs) in operando monitored by grazing-incidence X-ray diffraction (GIXRD). NaT2 maintains its monoclinic bulk motif in operating OFETs with a=20.31±0.06 Å, b=6.00±0.01 Å, c=8.17±0.04 Å and β=96.64±0.74°. Crystallites appear as a mosaic of single crystals reaching through the whole 50 nm thick active layer. The lattice parameters variation (<1%) falls within the statistical error of structure refinement when the OFET gate voltage is varied from 0 V to 40 V; or when the OFET is continuously cycled within this voltage interval over more than 10 h period. Within the first few cycles, both the hole mobility and threshold voltage are changing but then reach stable levels with an average mobility of ð3:25±0:04Þ 10^4 cm^2/Vs and an average threshold voltage of 13:6±0:2 V, both varying less than 4% for the remainder of the 10 h period. This demonstrates crystalline stability of NaT2 in operating OFETs.

General information
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Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, University of Southern Denmark, European Synchrotron Radiation Facility, Technical University of Denmark
Structure and Electrical Properties of NdBa$_2$Cu$_3$O$_y$ Thin Films by Laser Ablation at Low Oxygen Partial Pressure

A deposition process for NdBa$_2$Cu$_3$O$_y$ thin films by laser ablation at decreased deposition temperature was developed using substitution of oxygen with argon in the chamber during deposition. A low deposition rate is the crucial factor to obtain high-quality NBCO films. The Nd/Ba cation disorder in the film can be suppressed by an increase of the deposition temperature or by a decrease of the oxygen partial pressure during deposition. The presence of Nd/Ba disorder during deposition stimulates the introduction of oxygen into the growing film. A simple model is proposed for estimation of oxygen contents in the film using structural parameters measured with XRD techniques. Studies of the post-deposition annealing process showed ordering of the Nd/Ba sub-lattice and intense oxygen in- and out-diffusion. The temperature of the post-deposition annealing step should be chosen low enough (∼400 °C) to avoid oxygen diffusion out of the NBCO film.

General information
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Organisations: Department of Physics, Russian Academy of Sciences, Moscow Institute of Physics and Technology
Authors: Mozhaev, P. B. (Ekstern), Mozhaeva, J. (Intern), Khoryushin, A. (Intern), Puriy, A. V. (Ekstern), Hansen, J. O. B. (Ekstern), Jacobsen, C. S. (Intern)
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Scopus rating (2014): SJR 0.381 SNIP 0.613 CiteScore 0.86
Web of Science (2014): Indexed yes
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Scopus rating (2012): SJR 0.422 SNIP 0.496 CiteScore 0.64
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.443 SNIP 0.433 CiteScore 0.71
ISI indexed (2011): ISI indexed yes
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Scopus rating (2010): SJR 0.666 SNIP 0.409
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Structure sensitivity in the electrocatalytic reduction of CO$_2$ with gold catalysts

General information
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Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics, Technical University of Denmark, Imperial College London
Authors: Mezzavilla, S. (Intern), Duarte, R. (Ekstern), Maagaard, T. (Intern), Stephens, I. E. L. (Ekstern), Horch, S. (Intern), Seger, B. (Intern), Chorkendorff, I. (Intern)
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Studies of Deactivation of Methanol to Formaldehyde Selective Oxidation Catalyst

This work presents a study of the deactivation behavior of Fe-Mo oxide catalyst during selective oxidation of methanol to formaldehyde in a period of 5 days. The structural changes in the catalyst have been investigated in situ for the initial 10 h by Raman spectroscopy, and the structure after 5 days on stream in a fixed bed reactor have been determined by comprehensive characterization.

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Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, PILOT PLANT, Department of Physics, Experimental Surface and Nanomaterials Physics, Haldor Topsoe AS, Aarhus University, Karlsruhe Institute of Technology KIT
Authors: Raun, K. V. (Intern), Schumann, M. (Intern), Høj, M. (Intern), Thorhaug, M. (Ekstern), Beato, P. (Ekstern), Damsgaard, C. D. (Intern), Chevallier, J. (Forskerdatabase), Nielsen, K. (Intern), Grundwaldt, J. (Ekstern), Jensen, A. D. (Intern)
Number of pages: 2
Publication date: 2017
Event: Abstract from 13th European Congress on Catalysis (EUROPACAT 2017), Florence, Italy.
Main Research Area: Technical/natural sciences
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Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2017
Studies of Deactivation of Methanol to Formaldehyde Selective Oxidation Catalyst

Formaldehyde (CH2O) may be synthesized industrially by selective oxidation of methanol over an iron-molybdate (Fe-Mo) oxide catalyst according to: \( \text{CH}_3\text{OH} + \frac{1}{2}\text{O}_2 \rightarrow \text{CH}_2\text{O} + \text{H}_2\text{O} \). The reaction is normally carried out in a multitubular reactor with excess of air at 250-400 °C (yield = 90-95 %), known as the Formox process [1]. The average lifetime of the industrial catalyst is only 1–2 years depending on the operating conditions. The catalyst consists of a bulk phase of Fe2(MoO4)3 and a surface layer phase of MoO3. The MoO3 surface is selective towards formaldehyde while the iron in the sublayer increases the activity of the catalyst [2]. Pure MoO3 in itself has low activity. Literature from the last decades agrees that the major reason for the deactivation is loss of molybdenum from the catalyst. Molybdenum forms volatile species with methanol, which can leave behind Mo poor zones. The catalyst is usually prepared with excess MoO3 (\( \text{Mo/Fe} > 1.5 \)) to counter the loss of Mo. This work focuses on understanding the structural changes occurring in the catalyst and its behavior during deactivation via prolonged activity testing and spectroscopic investigations.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, PILOT PLANT, Department of Physics, Experimental Surface and Nanomaterials Physics, Haldor Topsoe AS, Aarhus University, Karlsruhe Institute of Technology KIT
Authors: Raun, K. V. (Intern), Schumann, M. (Ekstern), Hej, M. (Intern), Dalslet, B. T. (Ekstern), Beato, P. (Ekstern), Damsgaard, C. D. (Intern), Chevallier, J. (Ekstern), Grundwaldt, J. (Ekstern), Jensen, A. D. (Intern)
Number of pages: 1
Publication date: 2017
Main Research Area: Technical/natural sciences
Electronic versions:
NAM_25_Kristian_Raun.pdf

Sugar export limits size of conifer needles

Plant leaf size varies by more than three orders of magnitude, from a few millimeters to over one meter. Conifer leaves, however, are relatively short and the majority of needles are no longer than 6 cm. The reason for the strong confinement of the trait-space is unknown. We show that sugars produced near the tip of long needles cannot be exported efficiently, because the pressure required to drive vascular flow would exceed the greatest available pressure (the osmotic pressure). This basic constraint leads to the formation of an inactive region of stagnant fluid near the needle tip, which does not contribute to sugar flow. Remarkably, we find that the size of the active part does not scale with needle length. We predict a single maximum needle size of 5 cm, in accord with data from 519 conifer species. This could help rationalize the recent observation that conifers have significantly smaller leaves than angiosperms, and provide a biophysical explanation for this intriguing difference between the two largest groups of plants.

General information
State: Published
Organisations: Department of Physics, Biophysics and Fluids, University of California at Davis
Authors: Rademaker, H. (Intern), Zwieniecki, M. A. (Ekstern), Bohr, T. (Intern), Jensen, K. H. (Intern)
Number of pages: 1
Pages: 042402
Publication date: 2017
Main Research Area: Technical/natural sciences

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Journal: Physical Review E
Volume: 95
Issue number: 4
ISSN (Print): 2470-0045
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 0.987 SJR 0.979 CiteScore 2.14
Web of Science (2017): Indexed Yes
Scopus rating (2016): CiteScore 1.95 SJR 1.271 SNIP 1.018
Web of Science (2016): Indexed yes
Scopus rating (2015): SJR 1.183 SNIP 1.043 CiteScore 1.89
Sulfide perovskites for solar energy conversion applications: computational screening and synthesis of the selected compound LaYS$_3$

One of the key challenges in photoelectrochemical water splitting is to identify efficient semiconductors with band gaps of the order of ~2 eV to operate as the large-band-gap component in water splitting tandem devices. Here, we address this challenge by extensive computational screening of ternary sulfides followed by synthesis and confirmation of the properties of one of the most promising materials. The screening focusses on materials with ABS3 composition taking both perovskite and non-perovskite structures into consideration, and the material selection is based on descriptors for thermodynamic stability, light absorption, charge mobility, and defect tolerance. One of the most promising candidates identified is LaYS$_3$. This material was synthesized directly in thin-film form demonstrating its stability, crystal structure, light absorption, and strong photoluminescence. These data confirms its potential applicability in tandem photoelectrochemical devices for hydrogen production.
Surface theorem for the Chern-Simons axion coupling

The Chern-Simons axion coupling of a bulk insulator is only defined modulo a quantum of $e^2/h$. The quantized part of the coupling is uniquely defined for a bounded insulating sample, but it depends on the specific surface termination. Working in a slab geometry and representing the valence bands in terms of hybrid Wannier functions, we show how to determine that quantized part from the excess Chern number of the hybrid Wannier sheets located near the surface of the slab. The procedure is illustrated for a tight-binding model consisting of coupled quantum
anomalous Hall layers. By slowly modulating the model parameters it is possible to transfer one unit of Chern number from
the bottom to the top surface over the course of a cyclic evolution of the bulk Hamiltonian, changing the surface
anomalous Hall conductivity by a quantum of conductance $e^2/h$. When the evolution of the surface Hamiltonian is also
cyclic, the Chern pumping is obstructed by chiral touchings between valence and conduction surface bands.

General information
State: Published
Organisations: Department of Physics, Theoretical Atomic-scale Physics, ETH Zurich, Rutgers University, Universidad del
Pais Vasco
Authors: Olsen, T. (Intern), Taherinejad, M. (Ekstern), Vanderbilt, D. (Ekstern), Souza, I. (Ekstern)
Number of pages: 14
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Main Research Area: Technical/natural sciences

Publication information
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Volume: 95
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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
**Sustainable solar fuels and electricity through discovery and prototyping of new materials**

**General information**

State: Published
Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics, Silicon Microtechnology, Theoretical Atomic-scale Physics, Department of Micro- and Nanotechnology
Number of pages: 1
Publication date: 2017

**Host publication information**
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Publisher: Technical University of Denmark (DTU)
Main Research Area: Technical/natural sciences
Conference: Sustain 2017, Kgs. Lyngby, Denmark, 06/12/2017 - 06/12/2017
Electronic versions: SustainAbstracts2017c.compressed_115.pdf
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2017

**Swimming and feeding of mixotrophic biflagellates**

Many unicellular flagellates are mixotrophic and access resources through both photosynthesis and prey capture. Their fitness depends on those processes as well as on swimming and predator avoidance. How does the flagellar arrangement and beat pattern of the flagellate affect swimming speed, predation risk due to flow-sensing predators, and prey capture? Here, we describe measured flows around two species of mixotrophic, biflagellated haptophytes with qualitatively different flagellar arrangements and beat patterns. We model the near cell flows using two symmetrically arranged point forces with variable position next to a no-slip sphere. Utilizing the observations and the model we find that puller force arrangements favour feeding, whereas equatorial force arrangements favour fast and quiet swimming. We determine the capture rates of both passive and motile prey, and we show that the flow facilitates transport of captured prey along the haptonema structure. We argue that prey capture alone cannot fulfil the energy needs of the observed species, and that the mixotrophic life strategy is essential for survival.

**General information**

State: Published
Organisations: Department of Physics, Biophysics and Fluids, National Institute of Aquatic Resources, Centre for Ocean Life, Technical University of Denmark
Authors: Dölger, J. (Intern), Nielsen, L. T. (Intern), Kjærboe, T. (Intern), Andersen, A. P. (Intern)
Number of pages: 10
Publication date: 2017
Main Research Area: Technical/natural sciences

**Publication information**
Journal: Scientific Reports
Volume: 7
Article number: 39892
ISSN (Print): 2045-2322
Synthesis of Nanoparticle Model Systems for Sustainable Catalysis by Gas Aggregation

The overall goal of this thesis is to develop better catalysts for chemical reactions used in sustainable energy storage and environmental protection. Specifically, the thesis presents research on well-defined catalyst model systems of nanoparticles synthesized by magnetron sputtering, gas-aggregation, and subsequent mass-filtering. The thesis opens with a presentation of the broader context of the research, particularly focusing on the societal importance of catalysis, followed by an introduction to the fundamentals of the science of catalysis. Three research projects are then described in individual chapters, summarized in the following:

Platinum Catalysts for TW-Scale H2 Production: Platinum has the highest activity of known catalysts for the hydrogen evolution reaction (HER), but due to scarcity and price it is often assumed to be infeasible for photoelectrochemical water splitting on the terawatt-scale that is needed for significant global impact. This study investigates the relationship between catalytic activity for the HER and platinum catalyst loading using well-defined model systems with different loadings of mass-selected 5nm Pt nanoparticles. Using the knowledge gained on these systems, a technoeconomic analysis is carried out, showing that photoelectrochemical HER at a current density of 10 mA/cm² and an overpotential of 50mV could be obtained with a catalyst consumption of 54 tons of Pt per TW energy stored in H₂, corresponding to ~ 1/4 of the global, annual Pt production.

Synthesis of Ni−Mo−S Nanoparticles by Reactive Gas Aggregation: In this project, a method was developed for synthesizing in-flight sulfided Ni-Mo-S nanoparticles by aggregation of sputtered metal from a Mo₇₅Ni₂₅ target in a reactive atmosphere of Ar and H₂S. The resulting particles are undersulfided with a stoichiometry of Mo₀.₈Ni₀.₂S₁.₁, and the particles exhibit high-surface area morphologies such as platelets, very different from the spherical morphologies observed for metal nanoparticles. The particles are mass-filtered before deposition, and it is shown that different masses results in significantly different particle morphologies. Using a microreactor platform, the catalytic activity of the nanoparticles is assessed for hydrodesulfurization (HDS) of dibenzothiophene, relevant for e.g. production of diesel with ultra-low sulfur content. It is found that in-flight sulfided Ni-Mo-S nanoparticles have more than twice as high HDS activity as Ni-Mo-S nanoparticles produced by inert gas aggregation and post-sulfidation. This points towards the potential of
engineering nanoscale catalysts for HDS by reactive gas aggregation synthesis of nanoparticles.

**Dynamic Effects of Surface Oxygen in CO Electroreduction:** One of the keys to developing better catalysts for energy-storage by electrolysis of CO₂ is to understand the principles behind electroreduction of the reaction intermediate CO. This study reports the discovery of a high, transient production of methane at the onset of electroreduction of CO on mass-selected copper nanoparticles produced by inert gas-aggregation, investigated with a newly developed system for electrochemical mass-spectrometry. This “dynamic methane” is only observed when the nanoparticles have been exposed to O₂ before the electrode potential is stepped to CO-reduction potentials. Based on analysis of experimental data and density functional theory, it is proposed that the dynamic methane is formed on nanoparticle kink-sites, which are activated by adsorbed oxygen; the transient nature of the dynamic methane is attributed to the fact that the adsorbed oxygen is only metastable. The results contribute to the understanding of the role of oxygen in CO-electroreduction, and could potentially be used on industrial scale if metastable active sites were cyclically regenerated.

The presented research demonstrates the insights that can be gained by studying well-defined model systems in catalysis, which can both contribute to fundamental scientific understanding and guide the development of catalysis technology.

**General information**
State: Published
Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics
Authors: Bodin, A. (Intern), Chorkendorff, I. (Intern), Nielsen, J. H. (Intern)
Number of pages: 174
Publication date: 2017

**Publication information**
Publisher: Department of Physics, Technical University of Denmark
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions: PhD_thesis_Anders_Bodin_.pdf

**Relations**
Projects:
Synthesis of Nanoparticle Model Systems for Sustainable Catalysis by Gas Aggregation
Publication: Research › Ph.D. thesis – Annual report year: 2017

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**Technology for Si/CZTS Tandem Solar Cell**

**General information**
State: Published
Organisations: Department of Micro- and Nanotechnology, Silicon Microtechnology, Department of Physics, Experimental Surface and Nanomaterials Physics, DTU Danchip, Department of Photonics Engineering, Photovoltaic Materials and Systems
Authors: Hajijafarassar, A. (Intern), Crovetto, A. (Intern), Pedersen, T. (Intern), Mariño, S. L. (Intern), Schou, J. (Intern), Hansen, O. (Intern)
Number of pages: 1
Publication date: 2017

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Publisher: Technical University of Denmark (DTU)
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Main Research Area: Technical/natural sciences
Conference: Sustain 2017, Kgs. Lyngby, Denmark, 06/12/2017 - 06/12/2017
Electronic versions: SustainAbstracts2017c.compressed_127.pdf
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2017

**Technoscience as heritage in the classroom**
The heritage of the Technical University of Denmark (DTU) is not easily explained. There is a real temptation to blackbox the technology in itself. The History of Technology division is exploring ways to keep the box open and translate the workings of the technology and the explanations of the scientists. A study of the process of emergence, spread, impact and perhaps closure of the technology Flow Injection Analysis has been undertaken. It a story of multiplicity and it takes many twists and turns and includes a lot of difficult science. We decided to find a way to bring this story into the high-school classroom. The FIA technology is explained by letting the students explore and use a specific FIA machine in a virtual lab. We also wanted to introduce the findings in our historical exploration of FIA. This is done by telling the student several different narratives relating to FIA or other historical technoscience developments. The students work through one
or more scenarios and make decisions and debate. Our theory was, that they would use some of the apparatus they have gained from the narratives in the decision making process. In this talk I will revise the outcomes of this process.

**General information**
State: Published
Organisations: Department of Physics
Authors: Zwischer, L. (Intern)
Pages: 64-66
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Title of host publication: Education and Museum: Cultural Heritage and Learning: Final event and International Conference Proceedings
ISBN (Electronic): 978-88-909933-3-6
Main Research Area: Technical/natural sciences
Conference: Edmuse Conference, Rome, Italy, 26/06/2017 - 26/06/2017
Electronic versions:
Pages_from_Untitled_2.pdf
Source: PublicationPreSubmission
Source-ID: 13467843
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**Teknisk kulturarv i bogform**

**General information**
State: Published
Organisations: Department of Physics
Authors: Skyggebjerg, L. K. (Intern)
Publication date: 2017

**Publication information**
Source/Publisher: Teknologihistorie DTU
Main Research Area: Technical/natural sciences
Electronic versions:
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**Bibliographical note**
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Source: PublicationPreSubmission
Source-ID: 139067323
Publication: Communication › Internet publication – Annual report year: 2017

**TEM characterization of Ni-Ga intermetallic catalysts for hydrogenation of CO2**

**General information**
State: Published
Organisations: Center for Electron Nanoscopy, Department of Physics, Experimental Surface and Nanomaterials Physics
Authors: Spiga, C. (Intern), Silva, H. J. L. (Intern), Wagner, J. B. (Intern), Chorkendorff, I. (Intern), Damsgaard, C. D. (Intern)
Publication date: 2017
Main Research Area: Technical/natural sciences
Electronic versions:
Untitled.pdf
Source: PublicationPreSubmission
Source-ID: 133321458
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2017

**Temperature dependent photoreflectance study of Cu2SnS3 thin films produced by pulsed laser deposition**
The energy band structure of Cu2SnS3 (CTS) thin films fabricated by pulsed laser deposition was studied by photoreflectance spectroscopy (PR). The temperature-dependent PR spectra were measured in the range of T = 10–150 K. According to the Raman scattering analysis, the monoclinic crystal structure (C1c1) prevails in the studied CTS thin film; however, a weak contribution from cubic CTS (F-43m) was also detected. The PR spectra revealed the valence band splitting of CTS. Optical transitions at EA = 0.92 eV, EB = 1.04 eV, and EC = 1.08 eV were found for monoclinic CTS at
low-temperature (T = 10 K). Additional optical transition was detected at EAC = 0.94 eV, and it was attributed to the low-
temperature band gap of cubic CTS. All the identified optical transition energies showed a blueshift with increasing
temperature, and the temperature coefficient dE/dT was about 0.1 meV/K.

**General information**

State: Published
Organisations: Theoretical Atomic-scale Physics, Department of Micro- and Nanotechnology, Department of Physics, Experimental Surface and Nanomaterials Physics, Silicon Microtechnology, Department of Photonics Engineering, Optical Microsensors and Micromaterials, Tallinn University of Technology
Authors: Raadik, T. (Ekstern), Grossberg, M. (Ekstern), Krustok, J. (Ekstern), Kauk-Kuusik, M. (Ekstern), Crovetto, A. (Intern), Ettlinger, R. B. (Intern), Hansen, O. (Intern), Schou, J. (Intern)
Number of pages: 4
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Main Research Area: Technical/natural sciences

**Publication information**

Volume: 110
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Article number: 261105
ISSN (Print): 0003-6951
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BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): SNIP 1.167 SJR 1.382 CiteScore 3.25
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
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
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Physics: Condensed Matter
Volume: 29
Article number: 273002
ISSN (Print): 0953-8984
Ratings:
BFI (2018): BFI-level 1
Density functional theory, Molecular dynamics, Electronic structure theory

Electronic versions:
main.pdf. Embargo ended: 23/03/2018
The effect of dopants on grain growth and PL in CZTS nanoparticle thin films for solar cell applications

We have studied the effect of dopants such as Na, Sb, and Li in Cu2ZnSnS4 nanoparticle thin films [1]. The as-synthesized CZTS nanoparticles were inherently ligand-free [2], which allows the use of polar solvents, such as water and ethanol. Another advantage of these particles is that the user- and environmentally-friendly chloride salts can be directly dissolved in controllable amounts. This further circumvents the need for later incorporation of dopants, or a ligand-exchange step to functionalize the surface of the nanoparticles. In addition, the homogeneous distribution of additives in the ink allows uniform grain growth within the deposited absorber layer. By including Na in the nanoparticle ink, micron-sized grains throughout the whole absorber are achieved after annealing in a sulfur atmosphere at 600°C. The absorber layer appeared to be of full density, and no closed porosity could be detected. In addition, the photoluminescence signal increased by a factor of 200 after Na-inclusion. Without Na, the grains were very difficult to sinter, the film was porous, and the photoluminescence was low. This suggests that including Na reduces interface recombination in CZTS nanoparticle absorber layers. A concentration of Na/(Cu+Zn+Sn)=30% was necessary for the densification of the absorber, which is significantly higher than that used in other Na-doped CZTS systems. The annealed films were found to be of the desired Cu-poor and Zn-rich composition.

The Nordic Exhibition in 1888 – analyzed as a snapshot of the international exchange of knowledge and technology

General information
State: Published
Organisations: Department of Physics
Authors: Skyggebjerg, L. K. (Intern)
Number of pages: 1
Publication date: 2017
Event: Abstract from 25th International Congress of History of Science and Technology (ICHST), Rio de Janeiro, Brazil.
Main Research Area: Technical/natural sciences

Threat detection of liquid explosives and precursors from their x-ray scattering pattern using energy dispersive detector technology

Energy dispersive X-ray diffraction (EDXRD) can be applied for identification of liquid threats in luggage scanning in security applications. To define the instrumental design, the framework for data reduction and analysis and test the performance of the threat detection in various scenarios, a flexible laboratory EDXRD test setup was build. A data set of overall 570 EDXRD spectra has been acquired for training and testing of threat identification algorithms. The EDXRD data was acquired with limited count statistics and at multiple detector angles and merged after correction and normalization. Initial testing of the threat detection algorithms with this data set indicate the feasibility of detection levels of > 95% true positive with < 6% false positive alarms.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Department of Applied Mathematics and Computer Science, Image Analysis & Computer Graphics
Threat detection, Liquid threats, LAGs, EDXRD

Three-Dimensional Numerical Modeling of Acoustic Trapping in Glass Capillaries

Acoustic traps are used to capture and handle suspended microparticles and cells in microfluidic applications. A particular simple and much-used acoustic trap consists of a commercially available, millimeter-sized, liquid-filled straight glass capillary actuated by a piezoelectric transducer. Here, we present a three-dimensional numerical model of the acoustic pressure field in the liquid coupled to the displacement field of the glass wall, taking into account mixed standing and traveling waves as well as absorption. The model explains the dynamical mechanism that leads to the formation of localized acoustic resonance modes in such a straight acoustic waveguide without any geometrical cavities in the axial direction of the capillary. The model further predicts that some of these modes are well suited for acoustic trapping, and it provides estimates for their frequencies and quality factors, the magnitude of the acoustic radiation force on a single test particle as a function of position, and the resulting acoustic retention force of the trap. We show that the model predictions are in agreement with published experimental results, and we discuss how improved and more-stable acoustic-trapping modes might be obtained using the model as a design tool.

General information

State: Published
Organisations: Department of Physics, Biophysics and Fluids
Authors: Ley, M. W. H. (Intern), Bruus, H. (Intern)
Number of pages: 15
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information

Journal: Physical Review Applied
Volume: 8
Issue number: 2
Article number: 024020
ISSN (Print): 2331-7019
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BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 1.406 SJR 2.089 CiteScore 4.62
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
The physical properties of polycrystalline materials depend on their microstructure, which is the nano- to centimeter scale arrangement of phases and defects in their interior. Such microstructure depends on the shape, crystallographic phase and orientation, and interfacing of the grains constituting the material. This article presents a new non-destructive 3D technique to study centimeter-sized bulk samples with a spatial resolution of hundred micrometers: time-of-flight three-dimensional neutron diffraction (ToF 3DND). Compared to existing analogous X-ray diffraction techniques, ToF 3DND enables studies of samples that can be both larger in size and made of heavier elements. Moreover, ToF 3DND facilitates the use of complicated sample environments. The basic ToF 3DND setup, utilizing an imaging detector with high spatial and temporal resolution, can easily be implemented at a time-of-flight neutron beamline. The technique was developed and tested with data collected at the Materials and Life Science Experimental Facility of the Japan Proton Accelerator Complex (J-PARC) for an iron sample. We successfully reconstructed the shape of 108 grains and developed an indexing procedure. The reconstruction algorithms have been validated by reconstructing two stacked Co-Ni-Ga single crystals, and by comparison with a grain map obtained by post-mortem electron backscatter diffraction (EBSD).
Blob filaments are coherent structures in a turbulent plasma flow. Understanding the evolution of these structures is important to improve magnetic plasma confinement. Three state variables describe blob filaments in a plasma convection model. A dynamical systems approach analyzes the evolution of these three variables. A critical point of a variable defines a feature point for a region where that variable is significant. For a range of Rayleigh and Prandtl numbers, the bifurcations of the critical points of the three variables are investigated with time as the primary bifurcation parameter. Bifurcation curves separate the parameter planes into regions with different critical point configurations for the state variables. For Prandtl number equal to 1, the number of critical points of each state variable increases with increasing Rayleigh number. For Rayleigh number equal to 104, the number of critical points is the greatest for Prandtl numbers of magnitude 100.
Towards an integrated squeezed light source

Since its first generation more than 30 years ago, squeezed light has developed towards a tool for high precision measurements as well as a tool for quantum information tasks like quantum key distribution. Miniaturization of sensors is an active field of research with the prospect of many applications. The precision of optical sensors based on interferometric measurements is often limited by the fundamental shot noise. While shot noise can be reduced by increasing the employed light power, integrated sensors pose limitations on the maximum possible amount due to damaging effects of high intensity as well as power consumption. Bright quadrature squeezed light produced by the optical Kerr effect in a nonlinear medium offers an opportunity to overcome these limitations. Here, we present first steps towards a bright quadrature squeezed light source produced by the optical Kerr effect in race-track resonators in silicon nitride by presenting characterizations of the chip. Using standard fabrication techniques this source will have the potential of seamless integration into on-chip optical sensors.

General information
State: Published
Organisations: Department of Physics, Quantum Physics and Information Technology
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.

General information
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Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, Theoretical Atomic-scale Physics, Department of Physics, Neutrons and X-rays for Materials Physics, Experimental Surface and Nanomaterials Physics, Massachusetts Institute of Technology, SLAC National Accelerator Laboratory, Argonne National Laboratory, Oregon State University, University of Copenhagen
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BFI (2017): BFI-level 2
Scopus rating (2017): SNIP 4.819 SJR 14.59 CiteScore 30.87
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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
Transient flows in active porous media

Stimuli-responsive materials that modify their shape in response to changes in environmental conditions—such as solute concentration, temperature, pH, and stress—are widespread in nature and technology. Applications include micro- and nanoporous materials used in filtration and flow control. The physiochemical mechanisms that induce internal volume modifications have been widely studied. The coupling between induced volume changes and solute transport through porous materials, however, is not well understood. Here, we consider advective and diffusive transport through a small channel linking two large reservoirs. A section of stimulus-responsive material regulates the channel permeability, which is a function of the local solute concentration. We derive an exact solution to the coupled transport problem and demonstrate the existence of a flow regime in which the steady state is reached via a damped oscillation around the equilibrium concentration value. Finally, the feasibility of an experimental observation of the phenomena is discussed.
Translational, rotational, vibrational and electron temperatures of a gliding arc discharge

Translational, rotational, vibrational and electron temperatures of a gliding arc discharge in atmospheric pressure air were experimentally investigated using in situ, non-intrusive optical diagnostic techniques. The gliding arc discharge was driven by a 35 kHz alternating current (AC) power source and operated in a glow-type regime. The two-dimensional distribution of the translational temperature ($T_t$) of the gliding arc discharge was determined using planar laser-induced Rayleigh scattering. The rotational and vibrational temperatures were obtained by simulating the experimental spectra. The OH A–X (0, 0) band was used to simulate the rotational temperature ($T_{r}$) of the gliding arc discharge whereas the NO A–X (1, 0) and (0, 1) bands were used to determine its vibrational temperature ($T_v$). The instantaneous reduced electric field strength $E/N$ was obtained by simultaneously measuring the instantaneous length of the plasma column, the discharge voltage and the translational temperature, from which the electron temperature ($T_e$) of the gliding arc discharge was estimated. The uncertainties of the translational, rotational, vibrational and electron temperatures were analyzed. The relations of these four different temperatures ($T_e > T_v > T_r > T_t$) suggest a high-degree non-equilibrium state of the gliding arc discharge.
Tuning biomimetic membrane barrier properties by hydrocarbon, cholesterol and polymeric additives

The barrier properties of cellular membranes are increasingly attracting attention as a source of inspiration for designing biomimetic membranes. The broad range of potential technological applications makes the use of lipid and lately also polymeric materials a popular choice for constructing biomimetic membranes, where the barrier properties can be controlled by the composition of the membrane constituent elements. Here we investigate the membrane properties reported by the light-induced proton pumping activity of bacteriorhodopsin (bR) reconstituted in three vesicle systems of different membrane composition. Specifically we quantify how the resulting proton influx and efflux rates are influenced by the membrane composition using a variety of membrane modulators. We demonstrate that by adding hydrocarbons to vesicles with reconstituted bR formed from asolectin lipids the resulting transmembrane proton fluxes changes proportional to the carbon chain length when compared against control. We observe a similar proportionality in single-component 1,2-Dioleoyl-sn-glycero-3-phosphocholine (DOPC) model membranes when using cholesterol. Lastly we investigate the effects of adding the amphiphilic di-block co-polymer polybutadiene-polyethyleneoxide (PB\textsubscript{12}-PEO\textsubscript{10}) to phospholipid membranes formed from DOPC, 1,2-Dioleoyl-sn-glycero-3-phosphatidylethanolamine (DOPE), and 1,2-Dioleoyl-sn-glycero-3-phosphatidylserine (DOPS). The proton pumping activity of bR (measured as a change in extravesicular pH) in mixed lipid/PB\textsubscript{12}-PEO\textsubscript{10} lipid systems is up to six-fold higher compared to that observed for bR containing vesicles made from PB\textsubscript{12}-PEO\textsubscript{10} alone. Interestingly, bR inserts with apparent opposite orientation in pure PB12-PEO10 vesicles as compared to pure lipid vesicles. Addition of equimolar amounts of lipids to PB12-PEO10 results in bR orientation similar to that observed for pure lipids. In conclusion our results show how the barrier properties of the membranes can be controlled by the composition of the membrane. In particular the use of mixed lipid-polymer systems may pave the way for constructing biomimetic membranes tailored for optimal properties in various applications including drug delivery systems, biosensors and energy conservation technology.
Two-Dimensional MXenes as Catalysts for Electrochemical Hydrogen Evolution: A Computational Screening Study

We use density functional theory calculations to explore different polymorphs of a new class of 2D materials commonly known as MXenes, which are primarily carbides and nitrides of transition metals. The stability of the M$_2$X, M$_3$X$_2$, and M$_4$X$_3$ polymorphs in their bare and functionalized forms is assessed via the calculated standard heat of formation. We find that most of the MXenes are metallic, and we investigate their performance as electrocatalysts for the hydrogen evolution reaction (HER) using the free energy of hydrogen adsorption at equilibrium coverage as an activity descriptor. For a given type of metal, we find that the hydrogen adsorption energy can vary by up to 0.5 eV depending on the number of metal layers in the structure, suggesting that the catalytic activity of MXenes can be tuned by controlling the layer thickness. On the basis of a combined stability and activity analysis of 72 different MXenes, we identify several new promising nonprecious HER electrocatalysts.
Ultrafast dynamics of two copper bis-phenanthroline complexes measured by x-ray transient absorption spectroscopy:

Paper

Ultrafast structural dynamics of the metal to ligand charge transfer (MLCT) states of two copper bis-phenanthroline complexes were captured by using x-ray transient absorption (XTA) spectroscopy at the Linac Coherent Light Source and further described by theoretical calculations. These complexes have the general formula [Cu(I)(R)2]+, where R = 2,9-dimethyl-1,10-phenanthroline (dmp) and 2,9-diphenyl-1,10-phenanthroline disulfonic acid disodium salt (dpps).

[Cu(I)(dmp)2]2+ has methyl groups at the 2,9 positions of phenanthroline (phen) and adopts a pseudo-tetrahedral geometry. In contrast, [Cu(I)(dpps)2]2+ possesses two bulky phenyl-sulfonate groups attached to each phen ligand that force the molecule to adopt a flattened tetrahedral geometry in the ground state. Previously, optical transient absorption (OTA) and synchrotron based XTA experiments with 100 ps time resolution have been employed to study the relationship between structural distortions and excited state relaxation pathways in the two complexes. However, the dynamics of the MLCT transition during the first few picoseconds after excitation in these complexes remained unclear because of limitations in element specificity in OTA and in the time resolution of synchrotron sources in XTA.

In this experiment, the local coordination geometry and oxidation state of copper were probed with a temporal resolution of \( \sim 300 \) fs. Unexpectedly, the depletion of the Cu(I) signal due to the MLCT transition was found to be non-impulsive in the case of [Cu(I)(dpps)2]2+ with a time constant of 0.6 ps, while the Cu(I) depletion in [Cu(I)(dmp)2]2+ was instantaneous within the 300 fs instrument response time. The slower Cu(I) depletion kinetics in [Cu(I)(dpps)2]2+, previously unobserved in femtosecond OTA experiments, is likely due to intramolecular motions on the sub-picosecond time scale that could alter the localization of the transferred electron in the phen ligands.

General information

State: Published
Ultra-low-angle boundary networks within recrystallizing grains

We present direct evidence of a network of well-defined ultra-low-angle boundaries in bulk recrystallizing grains of 99.5% pure aluminium (AA1050) by means of a new, three-dimensional X-ray mapping technique; dark-field X-ray microscopy. These boundaries separate lattice orientation differences on the order of 0.05° and thus subdivide the recrystallizing grain into 2–7 μm wide domains. During further annealing the orientation differences decrease and the overall structure become more uniform while the network remains. It is observed that the morphology of the grain boundaries surrounding the recrystallizing grains relate to the intragranular network and effects hereof on the boundary migration is discussed.

General information
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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
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 2.314 SNIP 2.082 CiteScore 3.21
ISI indexed (2011): ISI indexed yes
Ultrasensitive and broadband magnetometry with cavity optomechanics
We achieved sensitivity of 30 pT/Hz$^{1/2}$ and working bandwidth larger than 100 MHz, using cavity optomechanical magnetometry, and also demonstrated quantum light enhanced sensitivity in such a magnetometer.

General information
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Organisations: Department of Physics, Quantum Physics and Information Technology, University of Queensland, Defense Science and Technology Group
Authors: Li, B. (Ekstern), Bulla, D. (Ekstern), Bilek, J. (Intern), Prakash, V. (Ekstern), Forstner, S. (Ekstern), Sheridan, E. (Ekstern), Madsen, L. (Ekstern), Rubinsztein-Dunlop, H. (Ekstern), Foster, S. (Ekstern), Schafermeier, C. (Intern), Gehring, T. (Intern), Andersen, U. (Intern), Bowen, W. (Ekstern)
Number of pages: 2
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Source: FindIt
Source-ID: 2392558232
Publication: Research - peer-review › Article in proceedings – Annual report year: 2017
Ultrasound Characterization of Microbead and Cell Suspensions by Speed of Sound Measurements of Neutrally Buoyant Samples

We present an experimental method including error analysis for the measurement of the density and compressibility of cells and microbeads; these being the two central material properties in ultrasound-based acoustophoretic applications such as particle separation, trapping, and up concentration. The density of the microparticles is determined by using a neutrally buoyant selection process that involves centrifuging of microparticles suspended in different density solutions, CsCl for microbeads and Percoll for cells. The speed of sound at 3 MHz in the neutrally buoyant suspensions is measured as a function of the microparticle volume fraction, and from this the compressibility of the microparticles is inferred. Finally, from the obtained compressibility and density, the acoustic scattering coefficients and contrast factor of the microparticles are determined, and in a sensitivity analysis, the impact of the measurement errors on the computed acoustic properties is reported. The determination of these parameters and their uncertainties allow for accurate predictions of the acoustophoretic response of the microparticles. The method is validated by determining the density (0.1-1% relative uncertainty) and compressibility (1-3% relative uncertainty) of previously well characterized polymer microbeads and subsequently applied to determine the density (0.1-1% relative uncertainty), compressibility (1% relative uncertainty), scattering coefficients, and acoustic contrast factors for nonfixed and fixed cells, such as red blood cells, white blood cells, DU-145 prostate cancer cells, MCF-7 breast cancer cells, and LU-HNSCC-25 head and-neck squamous carcinoma cells in phosphate buffered saline. The results show agreement with published data obtained by other methods.

General information
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Organisations: Department of Physics, Biophysics and Fluids, Lund University
Authors: Cushing, K. W. (Ekstern), Garofalo, F. (Ekstern), Magnusson, C. (Ekstern), Ekblad, L. (Ekstern), Bruus, H. (Intern), Laurell, T. (Ekstern)
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Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 6.08
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 6
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 5.79
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 6.01
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 5.8
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 5.86
ISI indexed (2011): ISI indexed yes
Ultrasound rays in droplets: The role of viscosity and caustics in acoustic streaming

When an acoustic wave propagates through a viscous fluid, it progressively transfers momentum to the fluid through viscous dissipation, which results in the formation of a steady vortical flow called acoustic streaming. Although spawned by viscous effects, the magnitude of the streaming does not depend on the viscosity in most simple geometries. However, viscosity has a profound influence on the acoustic streaming as demonstrated by Riaud et al. (J. Fluid Mech., vol. 821, 2017, pp. 384-420) in their study of sessile mm-sized water-glycerol droplets placed on a piezoelectric substrate with a 20-MHz ultrasound surface acoustic wave propagating along its surface. A detailed experimental and numerical analysis reveals that streaming dynamics is driven by a few ultrasound ray caustics inside the droplet.

General information
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Organisations: Department of Physics, Biophysics and Fluids
Authors: Bruus, H. (Intern)
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Scopus rating (2017): SJR 1.591 SNIP 1.702 CiteScore 3.33
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.82 SJR 1.744 SNIP 1.671
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.896 SNIP 1.639 CiteScore 2.57
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.864 SNIP 1.805 CiteScore 2.66
Web of Science (2014): Indexed yes
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.
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.

General information
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Organisations: Department of Applied Mathematics and Computer Science, Department of Energy Conversion and Storage, Imaging and Structural Analysis, Department of Physics, Neutrons and X-rays for Materials Physics, Universite Libre de Bruxelles, University of Rouen
Authors: Gbabode, G. (Ekstern), Delvaux, M. (Ekstern), Schweicher, G. (Ekstern), Andreasen, J. W. (Intern), Nielsen, M. M. (Intern), Geerts, Y. H. (Ekstern)
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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
Scopus rating (2007): SJR 3.1 SNIP 1.6
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 3.004 SNIP 1.72
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 2.623 SNIP 1.645
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 2.619 SNIP 1.693
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 2.565 SNIP 1.634
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 2.561 SNIP 1.7
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 2.863 SNIP 1.73
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 2.793 SNIP 2.012
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 2.75 SNIP 1.961
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Source: FindIt
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**Upconversion based spectral imaging in 6 to 8 μm spectral regime**

Spectral imaging in the 6 to 8μm range has great potential for medical diagnostics. Here a novel technique based on frequency upconversion of the infrared images to the near visible for subsequent acquisition using a Si-CCD camera is investigated. The upconversion unit consists of an AgGaS2 crystal and a 1064nm diode pumped solid state laser. A globar is used as mid-infrared illumination source. Acquired images contain both spectral and spatial information. Angle tuning of the nonlinear crystal is exploited to scan the phase match condition, which allows to cover the full spectral range of interest for the full field of view. Simulated images are created and compared with the measured images.
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.

Velocity-space sensitivities of neutron emission spectrometers at the tokamaks JET and ASDEX upgrade in deuterium plasmas

Future fusion reactors are foreseen to be heated by the energetic alpha particles produced in fusion reactions. For this to happen, it is important that the energetic ions are sufficiently confined. In present day fusion experiments, energetic ions are primarily produced using external heating systems such as neutral beam injection and ion cyclotron resonance heating. In order to diagnose these fast ions, several different fast-ion diagnostics have been developed and implemented in the various experiments around the world. The velocity-space sensitivities of fast-ion diagnostics are given by so-called weight functions. Here instrument-specific weight functions are derived for neutron emission spectrometry detectors at the tokamaks JET and ASDEX Upgrade for the 2.45 MeV neutrons produced in deuterium-deuterium reactions in deuterium plasmas. Using these, it is possible to directly determine which part of velocity space each detector observes.
Visualizing Catalysts in Action

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Authors: Damsgaard, C. D. (Intern)
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Source: PublicationPreSubmission
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Wake structure and thrust generation of a flapping foil in two-dimensional flow
We present a combined numerical (particle vortex method) and experimental (soap film tunnel) study of a symmetric foil undergoing prescribed oscillations in a two-dimensional free stream. We explore pure pitching and pure heaving, and contrast these two generic types of kinematics. We compare measurements and simulations when the foil is forced with pitching oscillations, and we find a close correspondence between flow visualisations using thickness variations in the soap film and the numerically determined vortex structures. Numerically, we determine wake maps spanned by oscillation frequency and amplitude, and we find qualitatively similar maps for pitching and heaving. We determine the drag–thrust transition for both pitching and heaving numerically, and we discuss it in relation to changes in wake structure. For heaving with low oscillation frequency and high amplitude, we find that the drag–thrust transition occurs in a parameter region with wakes in which two vortex pairs are formed per oscillation period, in contrast to the common transition scenario in regions with inverted von Kármán wakes.

General information
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Organisations: Department of Physics, Biophysics and Fluids, Department of Mechanical Engineering, Fluid Mechanics, Coastal and Maritime Engineering
Authors: Andersen, A. P. (Intern), Bohr, T. (Intern), Schnipper, T. (Intern), Walther, J. H. (Intern)
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What is the band alignment of Cu$_2$ZnSn(S,Se)$_4$ solar cells?

The band alignment at the Cu$_2$ZnSn(S,Se)$_4$/CdS solar cell heterojunction is a controversial issue, as different measurements and calculations point to substantially different conduction band offsets (CBO). As the actual value of the CBO has profound implications on solar cell performance, the aim of this work is to separate genuine process-dependent variations in the CBO from errors in its experimental determination. We argue that the two most likely mechanisms responsible for real CBO variations are Fermi level pinning (which tends to decrease the CBO) and chemical interdiffusion (which tends to increase the CBO). The experimental and computational approaches employed so far to determine the band alignment are analyzed to point out possible limitations for each approach, with an emphasis on photoemission-based approaches. The influence of Fermi level pinning on the CBO should be captured correctly by all types of measurements, except for measurements performed under flat-band conditions. This may explain some particularly large values of the CEO that have been measured under flat-band conditions. On the other hand, the influence of interdiffusion is difficult to resolve completely by most measurement approaches. Interestingly, a rough correlation can be established between the CBO measured at the Cu$_2$ZnSnS$_4$/CdS interface by different groups and their corresponding solar cell efficiency: lower-efficiency cells often have a large "cliff-like" offset, whereas most high-efficiency cells have a "spike-like" or nearly flat offset. Control of interdiffusion can be a powerful way to engineer the optimal band alignment in Cu$_2$ZnSnS$_4$/CdS solar cells, but it can be detrimental in Cu$_2$ZnSnSe$_4$/CdS solar cells, as it may increase the CBO above the optimal range for maximum efficiency.
Why iron oxide nanoflowers are great candidates for magnetic hyperthermia

General information
State: Published
Organisations: Department of Micro- and Nanotechnology, Magnetic Systems, Department of Physics, Neutrons and X-rays for Materials Physics, Universidad de Cantabria, Technische Universität Braunschweig, Physikalisch-Technische Bundesanstalt, Uppsala University, University College London, AGH University of Science and Technology, Chalmers University of Technology, Micromod Partikeltechnologie GmbH, Institut Laue-Langevin, RISE Acreo
Publication date: 2017
Event: Abstract from Nanomaterials Applied to Life Sciences 2017, Gijón, Spain.
Main Research Area: Technical/natural sciences
**X-ray diffraction microscopy based on refractive optics**

A formalism is presented for dark-field X-ray microscopy using refractive optics. The new technique can produce three-dimensional maps of lattice orientation and axial strain within millimetre-sized sampling volumes and is particularly suited to in situ studies of materials at hard X-ray energies. An objective lens in the diffracted beam magnifies the image and acts as a very efficient filter in reciprocal space, enabling the imaging of individual domains of interest with a resolution of 100 nm. Analytical expressions for optical parameters such as numerical aperture, vignetting, and the resolution in both direct and reciprocal spaces are provided. It is shown that the resolution function in reciprocal space can be highly anisotropic and varies as a function of position in the field of view. Inserting a square aperture in front of the objective lens facilitates disjunct and space-filling sampling, which is key for three-dimensional reconstruction and analysis procedures based on the conservation of integrated intensity. A procedure for strain scanning is presented. Finally the formalism is validated experimentally at an X-ray energy of 17 keV.

**General information**

State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, European Synchrotron Radiation Facility
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Main Research Area: Technical/natural sciences

**Publication information**

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Scopus rating (2017): SNIP 1.346 SJR 1.635 CiteScore 2.72
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
Zero-order filter for diffractive focusing of de Broglie matter waves

The manipulation of neutral atoms and molecules via their de Broglie wave properties, also referred to as de Broglie matter wave optics, is relevant for several fields ranging from fundamental quantum mechanics tests and quantum metrology to measurements of interaction potentials and new imaging techniques. However, there are several challenges. For example, for diffractive focusing elements, the zero-order beam provides a challenge because it decreases the signal contrast. Here we present the experimental realization of a zero-order filter, also referred to as an order-sorting aperture for de Broglie matter wave diffractive focusing elements. The zero-order filter makes it possible to measure even at low beam intensities.

We present measurements of zero-order filtered, focused, neutral helium beams generated at source stagnation pressures between 11 and 81 bars. We show that for certain conditions the atom focusing at lower source stagnation pressures (broader velocity distributions) is better than what has previously been predicted. We present simulations with the software ray-tracing simulation package MCSTAS using a realistic helium source configuration, which gives very good agreement with our measurements.

General information

State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, University of Bergen, University of Copenhagen, University of Genoa
Authors: Eder, S. D. (Ekstern), Ravn, A. K. (Ekstern), Samelin, B. (Ekstern), Bracco, G. (Ekstern), Salvador Palau, A. (Ekstern), Reisinger, T. (Ekstern), Bergbäck Knudsen, E. (Intern)
Number of pages: 5
Publication date: 2017
Main Research Area: Technical/natural sciences
A substrate and a method of using it
A substrate for a plurality of different measurement set-ups such as SERS, SPR and LSPR which substrate has a base and a plurality of elongate elements with metallic tips. A metallic layer is present on the base surface between the elongate elements and gaps or cavities exist between the layer and the tips or elongate elements. When the elongate elements and the base are transparent, transmission measurement set-ups are also possible.

General information
State: Published
Organisations: Department of Micro- and Nanotechnology, Department of Physics, Experimental Surface and Nanomaterials Physics, Nanoprobes, Center for Intelligent Drug Delivery and Sensing Using Microcontainers and Nanomechanics
Authors: Thilsted, A. H. (Intern), Schmidt, M. S. (Intern), Rindzevicius, T. (Intern), Boisen, A. (Intern)
Publication date: 5 Oct 2016

Publication information
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Patent number: EP3076161
Date: 05/10/2016
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Original language: English
Electronic versions:
Main Research Area: Technical/natural sciences
Source: espacenet
Source-ID: EP3076161
Publication: Research › Patent – Annual report year: 2016

A device for extracting volatile species from a liquid
The invention relates to a device (10) for extracting volatile species from a liquid (20) connected to an inlet of an analysis instrument, such as a mass spectrometer (MS). The device has a chamber (4), a membrane (5) forming a barrier for the liquid at zero differential pressure between the inside and the outside of the chamber, and allowing passage of the volatile species at zero differential pressure between the inside and the outside of the chamber. The device has an inlet capillary channel (3) to feed in a carrier gas and prevent back-diffusion from the chamber, and an outlet capillary channel (6) which provides a significant pressure reduction, e.g. from atmospheric pressure in the chamber (4) to near-vacuum suitable for an MS. The invention combines the best of two worlds, i.e. the fast time-response of a DEMS system and the high sensitivity of a MIMS system, since a differential pumping stage is not needed.

General information
State: Published
Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics, Department of Micro- and Nanotechnology, Silicon Microtechnology
Authors: Trimarco, D. B. (Intern), Vesborg, P. C. K. (Intern), Pedersen, T. (Intern), Hansen, O. (Intern), Chorkendorff, I. (Intern)
Publication date: 19 May 2016

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Date: 19/05/2016
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Original language: English
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Main Research Area: Technical/natural sciences
Source: espacenet
Source-ID: WO2016075208
30 years of squeezed light generation

Squeezed light generation has come of age. Significant advances on squeezed light generation have been made over the last 30 years—from the initial, conceptual experiment in 1985 till today’s top-tuned, application-oriented setups. Here we review the main experimental platforms for generating quadrature squeezed light that have been investigated in the last 30 years.

General information
State: Published
Organisations: Department of Physics, Quantum Physics and Information Technology, Friedrich-Alexander University Erlangen-Nuremberg
Authors: Andersen, U. L. (Intern), Gehring, T. (Intern), Marquardt, C. (Intern), Leuchs, G. (Ekstern)
Number of pages: 11
Publication date: 2016
Main Research Area: Technical/natural sciences

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Scopus rating (2017): CiteScore 1.14
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Scopus rating (2016): CiteScore 0.84
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 0.64
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 0.62
BFI (2013): BFI-level 1
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ISI indexed (2013): ISI indexed no
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Scopus rating (2012): CiteScore 0.67
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Web of Science (2012): Indexed yes
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Scopus rating (2011): CiteScore 0.85
ISI indexed (2011): ISI indexed no
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Web of Science (2006): Indexed yes
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Web of Science (2002): Indexed yes
Web of Science (2000): Indexed yes
Original language: English
Quantum optics, Squeezed light, Entanglement
Ab initio description of the thermoelectric properties of heterostructures in the diffusive limit of transport

The scope of this review is to present the recent progress in the understanding of the microscopic origin of thermoelectric transport in semiconducting heterostructures and to identify and elucidate mechanisms which could lead to enhanced thermoelectric conversion efficiency. Based on first-principles calculations a consistent and convenient method is presented to fully describe the thermoelectric properties in the diffusive limit of transport for bulk systems and their associated heterostructures. While fundamentals of the functionality of phonon-blocking and electron-transmitting superlattices could be unveiled, we provide also distinct analysis and ideas for thermoelectric enhancement for two archetypical thermoelectric heterostructures based on Bi$_2$Te$_3$/Sb$_2$Te$_3$ and Si/Ge. A focus was on the influence of bulk and interfacial strain, varying charge carrier concentration, temperature, and superlattice periods on the thermoelectric transport properties. Transmission electron micrograph of a 10 Å/50 Å Bi$_2$Te$_3$/ Sb$_2$Te$_3$ superlattice. Red and green areas highlight the layered structure. For optimal cross-plane transport (⊥) phonons (p) are expected to be scattered at the interfaces, while electrons (e$^-$) transmit without losses.

General information
State: Published
Organisations: Center for Atomic-scale Materials Design, Department of Physics, Martin-Luther-Universität, Helmholtz-Zentrum Dresden-Rossendorf, Max-Planck-Institut für Mikrostrukturphysik
Authors: Hinsche, N. F. (Intern), Rittweger, F. (Ekstern), Hölzer, M. (Ekstern), Zahn, P. (Ekstern), Ernst, A. (Ekstern), Mertig, I. (Ekstern)
Number of pages: 12
Pages: 672–683
Publication date: 2016
Main Research Area: Technical/natural sciences

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Scopus rating (2015): CiteScore 1.62
Web of Science (2015): Indexed yes
Scopus rating (2014): CiteScore 1.56
Web of Science (2014): Indexed yes
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ISI indexed (2013): ISI indexed yes
Scopus rating (2012): CiteScore 1.53
ISI indexed (2012): ISI indexed yes
Scopus rating (2011): CiteScore 1.66
ISI indexed (2011): ISI indexed yes
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Web of Science (2006): Indexed yes
Original language: English
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DOIs:
Acetaldehyde as an Intermediate in the Electroreduction of Carbon Monoxide to Ethanol on Oxide-Derived Copper

Oxide-derived copper (OD-Cu) electrodes exhibit unprecedented CO reduction performance towards liquid fuels, producing ethanol and acetate with >50% Faradaic efficiency at ~0.3 V (vs. RHE). By using static headspace-gas chromatography for liquid phase analysis, we identify acetaldehyde as a minor product and key intermediate in the electroreduction of CO to ethanol on OD-Cu electrodes. Acetaldehyde is produced with a Faradaic efficiency of ≈5% at ~0.33 V (vs. RHE). We show that acetaldehyde forms at low steady-state concentrations, and that free acetaldehyde is difficult to detect in alkaline solutions using NMR spectroscopy, requiring alternative methods for detection and quantification. Our results represent an important step towards understanding the CO reduction mechanism on OD-Cu electrodes.
Acetaldehyde as an Intermediate in the Electroreduction of Carbon Monoxide to Ethanol on Oxide-Derived Copper

Oxide-derived copper (OD-Cu) electrodes exhibit unprecedented CO reduction performance towards liquid fuels, producing ethanol and acetate with >50% Faradaic efficiency at −0.3 V (vs. RHE). By using static headspace-gas chromatography for liquid phase analysis, we identify acetaldehyde as a minor product and key intermediate in the electroreduction of CO to ethanol on OD-Cu electrodes. Acetaldehyde is produced with a Faradaic efficiency of ≈5% at −0.33 V (vs. RHE). We show that acetaldehyde forms at low steady-state concentrations, and that free acetaldehyde is difficult to detect in alkaline solutions using NMR spectroscopy, requiring alternative methods for detection and quantification. Our results represent an important step towards understanding the CO reduction mechanism on OD-Cu electrodes.
A compact two photon light sheet microscope for applications in neuroscience

We present a compact setup for two photon light sheet microscopy. By using pulsed Airy beam illumination we demonstrate eight-fold increase of the FOV compared to Gaussian light sheet with the same axial resolution.

General information
State: Published
Organisations: Department of Photonics Engineering, Diode Lasers and LED Systems, Department of Physics, Risø National Laboratory for Sustainable Energy, University of St Andrews, Femtolasers Produktions GmbH, Medical University of Vienna
Number of pages: 2
A comprehensive strategy for the analysis of acoustic compressibility and optical deformability on single cells

We realized an integrated microfluidic chip that allows measuring both optical deformability and acoustic compressibility on single cells, by optical stretching and acoustophoresis experiments respectively. Additionally, we propose a measurement protocol that allows evaluating the experimental apparatus parameters before performing the cell-characterization experiments, including a non-destructive method to characterize the optical force distribution inside the microchannel. The chip was used to study important cell-mechanics parameters in two human breast cancer cell lines, MCF7 and MDA-MB231. Results indicate that MDA-MB231 has both higher acoustic compressibility and higher optical deformability than MCF7, but statistical analysis shows that optical deformability and acoustic compressibility are not correlated parameters. This result suggests the possibility to use them to analyze the response of different cellular structures. We also demonstrate that it is possible to perform both measurements on a single cell, and that the order of the two experiments does not affect the retrieved values.
Acoustic Force Density Acting on Inhomogeneous Fluids in Acoustic Fields

We present a theory for the acoustic force density acting on inhomogeneous fluids in acoustic fields on time scales that are slow compared to the acoustic oscillation period. The acoustic force density depends on gradients in the density and compressibility of the fluid. For microfluidic systems, the theory predicts a relocation of the inhomogeneities into stable field-dependent configurations, which are qualitatively different from the horizontally layered configurations due to gravity. Experimental validation is obtained by confocal imaging of aqueous solutions in a glass-silicon microchip.
A DFT Structural Investigation of New Bimetallic PtSn\textsubscript{x} Surface Alloys Formed on the Pt(110) Surface and Their Interaction with Carbon Monoxide

Two surface alloys with \( p(3 \times 1) \) and \( p(6 \times 1) \) periodicity have been identified after the deposition of metallic Sn on the \( (1 \times 2) \)-Pt(110) surface. These two structures have been characterized by low energy electron diffraction (LEED), scanning tunneling microscopy (STM), and photoemission spectroscopy. Based on the experimental results and density functional theory (DFT) calculations, we propose atomic models for these surface alloys, which both consist of a highly corrugated row structure with a very similar surface motif. CO temperature-programmed desorption (TPD) experiments indicate that CO desorbs from the PtSn\textsubscript{x} surfaces at about 415-425 K compared to 495 K on the clean Pt(110). The energetics and geometry of the CO chemisorption sites have been studied by DFT calculations, obtaining an adsorption energy of 0.7-0.86 eV on \( p(3 \times 1) \) and 0.9-1.05 eV on \( p(6 \times 1) \). Overall our theoretical and experimental results indicate that the introduction of Sn strongly reduces the CO adsorption energy on the (110) oriented PtSn\textsubscript{x} surfaces.
Advanced microstructural analysis of cyclically deforming metallic materials towards lifetime improvement

General information
State: Published
Organisations: Department of Mechanical Engineering, Materials and Surface Engineering, Department of Physics, Neutrons and X-rays for Materials Physics, Deutsches Elektronen-Synchrotron
Authors: Diederichs, A. M. (Intern), Lienert, U. (Ekstern), Poulsen, H. F. (Intern), Pantleon, W. (Intern)
Number of pages: 1
Publication date: 2016
Main Research Area: Technical/natural sciences
Links:
http://www.sustain.dtu.dk/

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Advanced Neutron Moderators for the ESS
Thermal and cold neutrons are used in a wide array of different experiments investigating the sub-micrometer properties of matter. Neutrons are typically produced at reactor or spallation sources and subsequently cooled to the wanted thermal or cold energy levels by employing neutron moderators. The main increases in thermal and cold intensity are achieved by upscaling the power density of reactors or proton beam power of spallation sources. Reactor development saturated in the 1960s with the construction of the continuous, compact, high-power-density reactors HFIR, Oak Ridge, and ILL, Grenoble. Today these sources are still the most intense neutron sources. The short-pulsed sources SNS and J-PARC are the most powerful spallation sources in the world; although less intense than ILL and HFIR, these sources provide more useful neutrons because of their pulsed beam structure.

This thesis focuses on the European Spallation Source (ESS), which is currently being constructed in Lund, Sweden. The ESS will be a long-pulsed spallation source (pulse length 2.86 ms) driven by a 5-MW proton beam impinging on a rotating tungsten target. The ESS will be the world's most intense neutron source in terms of brightness, but it will also be the first spallation source to outperform reactors in terms of the integrated intensity of thermal and cold neutrons. Experiments at modern facilities use less than one millionth of the neutrons created in neutron source. Much of this inefficiency can be attributed to the moderator system. The imperfections of moderator systems originate from the highly isotropic slowing-down and thermalizing processes, premature leakage (fast neutron escape), neutron absorption and suboptimal geometrical configurations. The inefficiency of moderator systems implies a potential gain in efficiency for neutron sources, which generates an interest in moderator development. Many facilities have proposed and applied advanced moderator concepts to better utilize the produced neutrons. The topic of this thesis is the study of these advanced moderator concepts.

Chapters 1 to 6 briefly summarize the historical development of neutron sources. The ESS is briefly introduced. Then the governing physics is outlined as well as the main principles behind neutron sources and advanced moderators. Chapters 7 to 10 (further detailed below) present novel work in the form of three papers (two published articles, one submitted) and two conference proceedings.

Chapter 7 comprises two conference proceedings and describes the development from the moderator system at the ESS suggested in the Technical Design Report (TDR) to the new moderator baseline (accepted in March 2015), known as the butterfly moderator. The chapter outlines the development process from TDR through the pancake moderator and to the butterfly moderator, and presents various key results. Ultimately, it is shown how this redesign and optimization results in a significant increase in cold and thermal brightness relative to the TDR proposal.

Chapter 8 is a study in which MCNPX simulations are transferred to ROOT and analyzed. A method for reconstructing the full emission distribution of the moderator brightness is developed. The ESS pancake moderator (and butterfly moderator in the sub-appendix) is studied. The brightness distributions are fitted to analytical functions that have been implemented in McStas. This enables more precise predictions of the expectations from ESS, which is not only a key requirement for experiments at ESS but also enables neutron instruments to be significantly better optimized before their construction. This, in turn, is expected to contribute significantly to the overall quality of the ESS.

Chapter 9 suggests a novel type of broad-spectrum moderator. This moderator
The concept is based on the idea that heavy metals, such as lead and bismuth, are inefficient moderator materials. The article investigates this idea through enriched $^{208}$Pb. The article shows that the inability of these materials to moderate can be exploited to design a moderator that reflects neutrons from surrounding moderators of different spectral temperatures, with little change in energy. This results in the emission of a broad neutron spectrum (or multiple spectra) from the lead element. Since lead can also serve as a reflector filter, the geometry can be configured such that the broad-spectrum lead moderator acts as a reflector filter for a cold moderator positioned behind it, thus increasing the neutron yield below the lead Bragg edge whilst still producing a broad spectrum of neutrons.

Chapter 10 is an experimental paper carried out in the framework of the LENS collaboration. The experiment investigates the concept of a single-crystal reflector filter - a reflector filter that also transmits neutrons in the thermal energy range because of the delta-function-like Bragg edge in a single crystal. The experiment compares single-crystal sapphire, sapphire powder and void. Sapphire was used, since no other single-crystal candidates (diamond, pyrolytic graphite and lithium fluoride) could be obtained within the cost and time constraints of the experiment. Unfortunately, sapphire does not notably increase neutron yield, but the experiment proves the viability of a single-crystal reflector filter and indicates a potential regain of the thermal neutrons lost to a conventional reflector filter, with little or no loss of the cold neutrons below the Bragg edge.
A model for non-thermalized neutron spectra emitted from para-hydrogen
At spallation and reactor cold neutron sources, neutrons are cooled by moderators. At high power neutron sources, such as the Japan Proton Accelerator Research Complex (JPARC), European Spallation Source (ESS) and the Spallation Neutron Source (SNS) only few moderator materials are practical, due to the high radiation environment near the moderator and cooling demands. One of the very popular materials, used at J-PARC and planned for ESS, is the spin singlet state of H2, para-hydrogen. This study assesses the non-Maxwellian neutron spectral structure achieved in para-hydrogen moderators, which is due to the complexity of the inelastic scattering cross section below 50 meV. The analytical description of a thermalized spectrum with slowing down components are discussed, then a formula is developed which is a good description of this non-equilibrium para-hydrogen neutron spectrum. These analytical descriptions are fitted to the thermal and cold neutron spectra expected at the European Spallation Source according to the baseline configuration, as described in the Technical Design Report (TDR). The results of the fits have been implemented in McStas 2.0 and is used throughout the ESS instrumentation community. Though not shown here it is worth noting that the spectra for different heights of moderators in the more recent ESS geometry have also been fitted to this para-hydrogen spectrum model, the fits have been implemented and released in McStas 2.1.

General information
State: Published
Organisations: Center for Nuclear Technologies, Radiation Physics, Department of Physics, Neutrons and X-rays for Materials Physics, European Spallation Source ESS AB
Authors: Schönfeldt, T. (Intern), Batkov, K. (Ekstern), Klinkby, E. B. (Intern), Lauritzen, B. (Intern), Mezei, F. (Ekstern), Takibayev, A. (Ekstern), Willendrup, P. K. (Intern), Zanini, L. (Ekstern)
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Publisher: Japan Atomic Energy Agency
Editors: Oku, T., Nakamura, M., Sakai, K., Teshigawara, M., Tatsumoto, H., Yonemura, M., Suzuki, J., Arai, M.
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Number: 2015-002
Main Research Area: Technical/natural sciences
DOIs: 10.11484/jaea-conf-2015-002
Source: PublicationPreSubmission
Source-ID: 123117960
Publication: Research - peer-review › Article in proceedings – Annual report year: 2016

A multiple length scale description of the mechanism of elastomer stretching
Conventionally, the stretching of rubber is modeled exclusively by rotations of segments of the embedded polymer chains; i.e. changes in entropy. However models have not been tested on all relevant length scales due to a lack of appropriate probes. Here we present a universal X-ray based method for providing data on the structure of rubbers in the 2-50 angstrom range. First results relate to the elongation of a silicone rubber. We identify several non-entropic contributions to the free energy and describe the associated structural changes. By far the largest contribution comes from structural changes within the individual monomers, but among the contributions is also an elastic strain, acting between chains, which is 3-4 orders of magnitude smaller than the macroscopic strain, and of the opposite sign, i.e. extension of polymer chains in the direction perpendicular to the stretch. This may be due to trapped entanglements relaxing to positions close to the covalent crosslinks.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, The Danish Polymer Centre, Department of Physics, Neutrons and X-rays for Materials Physics, Oak Ridge National Laboratory, University of New South Wales, European Synchrotron Radiation Facility, Roskilde University
Authors: Neuefeind, J. (Ekstern), Skov, A. L. (Intern), Daniels, J. E. (Ekstern), Honkimaki, V. (Ekstern), Jakobsen, B. (Ekstern), Oddershede, J. (Intern), Poulsen, H. F. (Intern)
Pages: 95910-95919
Publication date: 2016
Main Research Area: Technical/natural sciences
An analytic mapping property of the Dirichlet-to-Neumann operator in Helmholtz boundary problems

The analytic version of microlocal analysis shows that if the boundary and the Dirichlet datum of a Helmholtz boundary value problem are real-analytic, then so is the corresponding Neumann datum. However, the domain of analytic continuation of the Neumann datum is, in general, unknown. We shall here relate, in terms of explicit estimates, the domains of analytic continuation of Dirichlet and Neumann boundary data for Helmholtz problems in two or more independent variables, and in neighbourhoods of planar pieces of the boundary. For this purpose, we shall characterise a special subspace of the standard pseudodifferential operators with real-analytic symbols, to which the Dirichlet-to-Neumann operator belongs. The result can be applied in the estimation of the domain of analytic continuation of solutions across planar pieces of the boundary.

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, Neutrons and X-rays for Materials Physics
Authors: Karamehmedovic, M. (Intern)
Number of pages: 1
Publication date: 2016
Main Research Area: Technical/natural sciences
Electronic versions: abstracts.pdf
A Spectral Geometrical Model for Compton Scatter Tomography Based on the SSS Approximation
The forward model of single scatter in the Positron Emission Tomography for a detector system possessing an excellent spectral resolution under idealized geometrical assumptions is investigated. This model has the form of integral equations describing a flux of photons emanating from the same annihilation event and undergoing a single scattering at a certain angle. The equations for single scatter calculation are derived using the Single Scatter Simulation approximation. We show that the three-dimensional slice-by-slice filtered backprojection algorithm is applicable for scatter data inversion provided some assumptions on the attenuation map are justified.

General information
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Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Department of Applied Mathematics and Computer Science, Scientific Computing, Institute of Computational Mathematics and Mathematical Geophysics
Authors: Kazantsev, I. G. (Ekstern), Olsen, U. L. (Intern), Poulsen, H. F. (Intern), Hansen, P. C. (Intern)
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Main Research Area: Technical/natural sciences

Atomically Thin Ordered Alloys of Transition Metal Dichalcogenides: Stability and Band Structures
We explore the possibility of modulating the electronic band edges of the transition metal dichalcogenides (TMD) via alloying of different semiconductors within the same group (intra-group alloying). The stability of the ordered alloys is assessed from the calculated mixing enthalpy which is found to be close to zero for several alloys and below 20 meV/atom for all the alloys. We explore to what extent the electronic properties like the band gap and band edge positions of the alloy can be evaluated by taking the weighted average of the corresponding properties of the pristine systems. In general, this approach works well with the only exception being Cr containing compounds. Because the calculated properties of the alloys are very similar to the weighted averages, we expect that the trends observed for the ordered alloys will also hold for more realistic disordered alloys.

General information
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Organisations: Center for Atomic-scale Materials Design, Department of Physics, Center for Nanostructured Graphene
Authors: Pandey, M. (Intern), Jacobsen, K. W. (Intern), Thygesen, K. S. (Intern)
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Main Research Area: Technical/natural sciences

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Scopus rating (2017): SJR 2.135 SNIP 1.147 CiteScore 4.58
Web of Science (2017): Indexed yes
Atomic scale analysis of sterical effects in the adsorption of 4,6-dimethyldibenzothiophene on a CoMoS hydrotreating catalyst

The low catalytic hydrodesulfurization (HDS) activity toward sterically hindered sulfur-containing molecules is a main industrial challenge in order to obtain ultra-low sulfur diesel. In this study we report a combined Scanning Tunneling Microscopy (STM) and Density Functional Theory (DFT) investigation of the adsorption of the sterically hindered sulfur-containing molecule 4,6-dimethyldibenzothiophene (4,6-DMDBT) onto a hydrotreating model catalyst for the Co promoted MoS2 (CoMoS) phase. The molecular adsorption occurs exclusively on the Co-promoted S-edge, most predominantly in a precursor-like diffusive physisorption referred to as delocalized π-mode. 4,6-DMDBT adsorption directly in a S-edge sulfur vacancy is observed exclusively in S-edge corner vacancies in an adsorption configuration reflecting a σ-coordination. STM movies reveal dynamic conversion between the σ-mode and an on-top π-adsorption providing a link between different adsorption sites and hence between the hydrogenation and direct desulfurization pathways in HDS. The low overall direct desulfurization activity of 4,6-DMDBT and related molecules is consistent with the low occurrence of S-...
vacancies on CoMoS S-edges predicted under HDS conditions in this study.

**General information**
State: Published
Organisations: Center for Atomic-scale Materials Design, Department of Physics, Theoretical Atomic-scale Physics, Aarhus University, Haldor Topsoe AS, University of Copenhagen
Authors: Grønborg, S. S. (Ekstern), Šaric, M. (Intern), Moses, P. G. (Ekstern), Rossmeisl, J. (Ekstern), Lauritsen, J. V. (Ekstern)
Number of pages: 8
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Scopus rating (2017): SNIP 1.85 SJR 2.397 CiteScore 6.99
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BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 7.27 SJR 2.451 SNIP 2.142
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 2.668 SNIP 2.177 CiteScore 7.23
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.688 SNIP 2.233 CiteScore 6.92
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.553 SNIP 2.091 CiteScore 6.42
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 3.006 SNIP 2.257 CiteScore 6.17
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 3.092 SNIP 2.214 CiteScore 6.23
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 3.38 SNIP 2.193
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.965 SNIP 2.135
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 3.123 SNIP 2.164
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 3.15 SNIP 2.138
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 3.137 SNIP 2.043
Web of Science (2006): Indexed yes
Atomic-Scale Analysis of the RuO₂/Water Interface under Electrochemical Conditions

The structure of the interface between ruthenium oxide and water was examined using density functional theory calculations for a range of pH and electrode potential values, and the results were summarized in a surface Pourbaix diagram. The results indicate that pH affects the interfacial structure as a consequence of the formation of a stable hydrogen network and the impact of the electric field on the interfacial Gibbs energy. Focusing on the potential region of the oxygen evolution reaction (1.23 V vs a reversible hydrogen electrode (RHE) + overpotential), variations in pH were found to change both the formal Ru valency and the structure of the primary water layer by altering the work function of the interfacial structure. We hypothesize that the effects of pH on the hydrogen bond network and formal valency observed in this work also apply to other transition-metal oxides.

General information

State: Published
Organisations: Center for Atomic-scale Materials Design, Department of Physics, University of Tokyo
Authors: Watanabe, E. (Ekstern), Rossmeisl, J. (Intern), Björketun, M. (Intern), Ushiyama, H. (Ekstern), Yamashita, K. (Ekstern)
Number of pages: 8
Pages: 8096-8103
Publication date: 2016
Main Research Area: Technical/natural sciences

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Volume: 120
Issue number: 15
ISSN (Print): 1932-7447
Ratings:
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SJR 2.135 SNIP 1.147 CiteScore 4.58
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
Atomic-scale Modelling of Electro-catalytic Surfaces and Dynamic Electrochemical Interfaces

This dissertation addresses numerical calculations on the atomic scale to study catalytic surfaces for electrochemistry. The first half of the thesis deals with calculations on the properties of catalytic surfaces, using well known methodology, whereas the second half of the thesis deals with the development of new methodology to explicitly include the electrolyte in the atomic scale calculations.

Chapter 3 presents calculations on contracted and reconstructed platinum surfaces, which are relevant for development of catalysts for proton exchange membrane fuel cells. Correlation of the results with experimental observations show that there is a natural limit to how far the reactivity of the catalysts can can be fine-tuned, exclusively using the strain effect, that is imposed by alloying with lanthanides.

In chapter 4, calculations are presented for several newly discovered catalysts for the hydrogen evolution reaction. The results show that molybdenum carbides and borides have reactive surfaces, which is not in consistency with their high catalytic activity. A possible active facet is suggested for the molybdenum boride. It is likely, however, that other unexplored active sites, surface terminations or phases are responsible for the observed catalytic activities. For nickel diphasphide, which is another recently discovered catalyst for the hydrogen evolution reaction, it was possible to determine several facets and active sites, which have advantageous catalytic properties.

Chapter 5 presents the new methodology to calculate the structure of the electrolyte in the electrochemical interface. The strength of this methodology is that it makes fewer assumptions on the physics of the interface, while it takes a fundamental statistical mechanics approach. Large datasets of states for the electrolyte in contact with the surfaces of gold (111) and platinum (111) were calculated. Analysis methods were developed for determining the structure of the
electrolyte as averages, which depend on pH and the electrode potential of the metal. The methodology remains under development, and it is expected that it will contribute with new insight to how pH and ionic chemical potentials affect the structure of the interface, to the benefit of future fundamental research in electrochemistry.

**General information**

State: Published

Organisations: Department of Physics, Theoretical Atomic-scale Physics

Authors: Hansen, M. H. (Intern), Thygesen, K. S. (Intern), Rossmeisl, J. (Intern)

Number of pages: 287

Publication date: 2016

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Main Research Area: Technical/natural sciences

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**Relations**

Projects:

Atomistic modelling of electro-catalytic surfaces and dynamic electrochemical interfaces

Publication: Research › Ph.D. thesis – Annual report year: 2016

**Atomistic characterization of the active-site solvation dynamics of a model photocatalyst**

The interactions between the reactive excited state of molecular photocatalysts and surrounding solvent dictate reaction mechanisms and pathways, but are not readily accessible to conventional optical spectroscopic techniques. Here we report an investigation of the structural and solvation dynamics following excitation of a model photocatalytic molecular system $[\text{Ir}_2(\text{dimen})_4]^{2+}$, where dimen is para-diisocyanomenthane. The time-dependent structural changes in this model photocatalyst, as well as the changes in the solvation shell structure, have been measured with ultrafast diffuse X-ray scattering and simulated with Born-Oppenheimer Molecular Dynamics. Both methods provide direct access to the solute-solvent pair distribution function, enabling the solvation dynamics around the catalytically active iridium sites to be robustly characterized. Our results provide evidence for the coordination of the iridium atoms by the acetonitrile solvent and demonstrate the viability of using diffuse X-ray scattering at free-electron laser sources for studying the dynamics of photocatalysis.

**General information**

State: Published

Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Department of Chemistry, Stanford University, SLAC National Accelerator Laboratory, Jan Kochanowski University, Korea Advanced Institute of Science & Technology, Inha University, Lund University


Number of pages: 35

Publication date: 2016

Main Research Area: Technical/natural sciences

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Web of Science (2018): Indexed yes

BFI (2017): BFI-level 2

Scopus rating (2017): CiteScore 12.41 SJR 6.582 SNIP 2.912

Web of Science (2017): Indexed yes

BFI (2016): BFI-level 2

Scopus rating (2016): CiteScore 11.8 SJR 6.414 SNIP 2.855

Web of Science (2016): Indexed yes

BFI (2015): BFI-level 1
A two-stage model of rough-interface scattering for embedded nano-structures

We decompose scattering by nanostructures on rough substrates into two surface transfer functions: one heuristic, computed for the bare substrate from experimental BRDF data, and the other sparse and constructed for nanostructures on smooth surfaces. We explore numerically the performance and the commutativity of this approach.

A Web Based Approach to Model Efficiencies of Solar Fuels Devices

General information
State: Published
Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics, Department of Micro- and Nanotechnology, Silicon Microtechnology
Back-illuminated Si-based photoanode with nickel cobalt oxide catalytic protection layer

Si is an excellent photo-absorber for use in dual-band-gap photoelectrochemical water splitting. We investigate photoanodes with n⁺p⁺-Si configuration under back-side illumination, which is suited to work in a tandem device stack. A co-sputtered NiCoOₓ film coupled to the Si was used as a protective catalyst for the water oxidation reaction in 1 m KOH. The sample showed a high photocurrent (21 mA cm⁻²) under red-light illumination (38.6 mW cm⁻²). Long-term stability testing showed a gradual decrease of activity in the beginning, and then the activity increased, yielding a cathodic shift of the onset voltage (>50 mV), likely owing to the divergent response of Ni and Co to the Fe present in KOH. Once the activity of the sample stabilized, no further degradation was observed for the following 6 days, indicating that the demonstrated back-illuminated photoanode configuration can be considered a promising architecture for use as a bottom cell of the tandem water-splitting device under alkaline conditions.
Band Gap Tuning and Defect Tolerance of Atomically Thin Two-Dimensional Organic-Inorganic Halide Perovskites

Organic–inorganic halide perovskites have proven highly successful for photovoltaics but suffer from low stability, which deteriorates their performance over time. Recent experiments have demonstrated that low dimensional phases of the hybrid perovskites may exhibit improved stability. Here we report first-principles calculations for isolated monolayers of the organometallic halide perovskites (C₄H₉NH₃)₂MX₂Y₂, where M = Pb, Ge, Sn and X, Y = Cl, Br, I. The band gaps computed using the GLLB-SC functional are found to be in excellent agreement with experimental photoluminescence data for the already synthesized perovskites. Finally, we study the effect of different defects on the band structure. We find that the most common defects only introduce shallow or no states in the band gap, indicating that these atomically thin 2D perovskites are likely to be defect tolerant.

General information
State: Published
Organisations: Department of Physics, Theoretical Atomic-scale Physics, Center for Nanostructured Graphene
Authors: Pandey, M. (Intern), Jacobsen, K. W. (Intern), Thygesen, K. S. (Intern)
Pages: 4346-4352
Publication date: 2016
Main Research Area: Technical/natural sciences

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Journal: Journal of Physical Chemistry Letters
Volume: 7
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BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): SNIP 1.595 SJR 4.667 CiteScore 8.37
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 8.18 SJR 4.602 SNIP 1.651
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 4.143 SNIP 1.758 CiteScore 8.04
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 3.725 SNIP 1.71 CiteScore 7
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 3.529 SNIP 1.608 CiteScore 6.61
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 3.965 SNIP 1.742 CiteScore 6.3
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 3.283 SNIP 1.613 CiteScore 5.95
ISI indexed (2011): ISI indexed no
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Web of Science (2010): Indexed yes
Web of Science (2009): Indexed yes
Web of Science (2008): Indexed yes
Web of Science (2007): Indexed yes
Web of Science (2006): Indexed yes
Web of Science (2005): Indexed yes
Benchmark and combined velocity-space tomography of fast-ion D-alpha spectroscopy and collective Thomson scattering measurements

We demonstrate the combination of fast-ion D-alpha spectroscopy (FIDA) and collective Thomson scattering (CTS) measurements to determine a common best estimate of the fast-ion velocity distribution function by velocity-space tomography. We further demonstrate a benchmark of FIDA tomography and CTS measurements without using a numerical simulation as common reference. Combined velocity-space tomographies from FIDA and CTS measurements confirm that sawtooth crashes reduce the fast-ion phase-space densities in the plasma center and affect ions with pitches close to one more strongly than those with pitches close to zero.

General information
State: Published
Organisations: Department of Physics, Plasma Physics and Fusion Energy, Max Planck Institute for Plasma Physics
Authors: Jacobsen, A. S. (Intern), Salewski, M. (Intern), Geiger, B. (Ekstern), Korsholm, S. B. (Intern), Leipold, F. (Intern), Nielsen, S. K. (Intern), Rasmussen, J. (Intern), Pedersen, M. S. (Intern), Weiland, M. (Ekstern)
Number of pages: 5
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 1.243 SJR 0.69 CiteScore 1.74
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1 SJR 1.433 SNIP 1.258
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.314 SNIP 1.345 CiteScore 1.1
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.542 SNIP 1.346 CiteScore 1.61
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.2 SNIP 1.253 CiteScore 1.54
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.453 SNIP 1.201 CiteScore 1.63
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
Reverse osmosis (RO)-based desalination and wastewater reclamation are gaining increasing popularity driven by water shortages and population growth. Advances in membrane technology in the past few decades have resulted in great savings in energy consumption of RO processes. Further reduction in energy consumption calls for novel membranes with significantly enhanced water permeability compared to the current state of the art thin-film composite polyamides. An attractive option is to learn from nature’s high efficiently water filtration systems that involve a group of specialised water transport proteins - aquaporins. This chapter presents the recent development of aquaporin-based biomimetic membranes, a topic that received a great interest in the membrane community in recent years.
This paper reports on a bi-resonant structure of piezoelectric PVDF films energy harvester (PPEH), which consists of two cantilevers with resonant frequencies of 15 Hz and 22 Hz. With increased acceleration, the vibration amplitudes of the two cantilever-mass structures are increased and collision occurs which causes strong mechanical coupling between the two subsystems. The experimental results show that the operating bandwidth is widened to 14 Hz (14–28 Hz) at an acceleration of 9.81 m/s², and the peak output power can be 0.35 W at a relatively low operation frequency of 16 Hz. Simulation and experiments with piezoelectric elements show that the energy harvesting device with the bi-resonant structure can generate higher power output than that of the sum of the two separate devices from random vibration sources at low frequency, and hence significantly improves the vibration-to-electricity conversion efficiency by 40–81%.
Black silicon solar cells with black bus-bar strings

We present the combination of black silicon texturing and blackened bus-bar strings as a potential method for obtaining all-black solar panels, while using conventional, front-contacted solar cells. Black silicon was realized by maskless reactive ion etching resulting in total, average reflectance below 0.5% across a 156x156 mm2 silicon wafer. Four different methods to obtain blackened bus-bar strings were compared with respect to reflectance, and two of these methods (i.e., oxidized copper and etched solder) were used to fabricate functional all-black solar 9-cell panels. The black bus-bars (e.g., by oxidized copper) have a reflectance below 3% in the entire visible wavelength range. The combination of black silicon cells and blackened bus-bars results in aesthetic, all-black panels based on conventional, front-contacted solar cells without compromising efficiency.

General information
State: Published
Organisations: Department of Micro- and Nanotechnology, Silicon Microtechnology, Department of Photonics Engineering, Diode Lasers and LED Systems, Experimental Surface and Nanomaterials Physics, Institute for Product Development, Gaia Solar A/S, Institute for Energy Technology
Authors: Davidsen, R. S. (Intern), Tang, P. T. (Ekstern), Mizushima, I. (Ekstern), Thorsteinsson, S. (Intern), Poulsen, P. B. (Intern), Frausig, J. (Ekstern), Nordseth, Ø. (Ekstern), Hansen, O. (Intern)
Number of pages: 4
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Source-ID: 125199253
Publication: Research - peer-review » Article in proceedings – Annual report year: 2016
Black silicon solar cells with black bus-bar strings

**General information**
State: Published
Organisations: Department of Micro- and Nanotechnology, Silicon Microtechnology, Department of Photonics Engineering, Diode Lasers and LED Systems, Experimental Surface and Nanomaterials Physics, Institute for Product Development, Gaia Solar A/S, Institute for Energy Technology
Authors: Davidsen, R. S. (Intern), Tang, P. T. (Ekstern), Mizushima, I. (Ekstern), Thorsteinsson, S. (Intern), Poulsen, P. B. (Intern), Frausig, J. (Ekstern), Nordseth, Ø. (Ekstern), Hansen, O. (Intern)
Number of pages: 1
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Main Research Area: Technical/natural sciences
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**Bibliographical note**
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Source: PublicationPreSubmission
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Publication: Research › Poster – Annual report year: 2016

**Black Silicon Solar Cells with Black Ribbons.**
We present the combination of mask-less reactive ion etch (RIE) texturing and blackened interconnecting ribbons as a method for obtaining all-black solar panels, while using conventional, front-contacted solar cells. Black silicon made by mask-less reactive ion etching has total, average reflectance below 0.5% across a 156x156 mm2 silicon (Si) wafer. Black interconnecting ribbons were realized by oxidizing copper resulting in reflectance below 3% in the visible wavelength range. Screen-printed Si solar cells were realized on 156x156 mm2 black Si substrates with resulting efficiencies in the range 15.7-16.3%. The KOH-textured reference cell had an efficiency of 17.9%. The combination of black Si and black interconnecting ribbons may result in aesthetic, all-black panels based on conventional, front-contacted silicon solar cells.

**General information**
State: Published
Organisations: Department of Micro- and Nanotechnology, Silicon Microtechnology, Department of Photonics Engineering, Diode Lasers and LED Systems, Experimental Surface and Nanomaterials Physics, Institute for Product Development, Gaia Solar A/S, Institute for Energy Technology
Authors: Davidsen, R. S. (Intern), Tang, P. T. (Ekstern), Mizushima, I. (Ekstern), Thorsteinsson, S. (Intern), Poulsen, P. B. (Intern), Frausig, J. (Ekstern), Nordseth, Ø. (Ekstern), Hansen, O. (Intern)
Number of pages: 4
Publication date: 2016

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Main Research Area: Technical/natural sciences
Conference: 32nd European Photovoltaic Solar Energy Conference and Exhibition, Munich, Germany, 20/06/2016 - 20/06/2016
Black Silicon, Nanostructuring, BIPV, Aesthetics, Inorganic Black Ribbons

**Bibliographical note**
Proceedings manuscript for EU PVSEC 2016 conference, Munich, Germany
Source: PublicationPreSubmission
Source-ID: 125199272
Publication: Research - peer-review › Article in proceedings – Annual report year: 2016

**Black silicon with black bus-bar strings**
We present the combination of black silicon texturing and blackened bus-bar strings as a potential method for obtaining all-black solar panels, while using conventional, front-contacted solar cells. Black silicon was realized by mask-less reactive ion etching resulting in total, average reflectance below 0.5% across a 156x156 mm2 silicon wafer. Black bus-bars were realized by oxidized copper resulting in reflectance below 3% in the entire visible wavelength range. The combination of these two technologies may result in aesthetic, all-black panels based on conventional, front-contacted solar cells without compromising efficiency.
Blob dynamics in the TORPEX experiment: a multi-code validation

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Main Research Area: Technical/natural sciences

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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 1.243 SJR 0.69 CiteScore 1.74
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1 SJR 1.433 SNIP 1.258
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.314 SNIP 1.345 CiteScore 1.1
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.542 SNIP 1.346 CiteScore 1.61
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.2 SNIP 1.253 CiteScore 1.54
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Blue emitting organic semiconductors under high pressure: status and outlook

This review describes essential optical and emerging structural experiments that use high GPa range hydrostatic pressure to probe physical phenomena in blue-emitting organic semiconductors including π-conjugated polyfluorene and related compounds. The work emphasizes molecular structure and intermolecular self-organization that typically determine transport and optical emission in π-conjugated oligomers and polymers. In this context, hydrostatic pressure through diamond anvil cells has proven to be an elegant tool to control structure and interactions without chemical intervention. This has been highlighted by high pressure optical spectroscopy whilst analogous x-ray diffraction experiments remain less frequent. By focusing on a class of blue-emitting π-conjugated polymers, polyfluorenes, this article reviews optical spectroscopic studies under hydrostatic pressure, addressing the impact of molecular and intermolecular interactions on optical excitations, electron-phonon interaction, and changes in backbone conformations. This picture is connected to the optical high pressure studies of other π-conjugated systems and emerging x-ray scattering experiments from polyfluorenes which provides a structure-property map of pressure-driven intra- and interchain interactions. Key obstacles to obtain further advances are identified and experimental methods to resolve them are suggested.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, University of Missouri
Authors: Knaapila, M. (Intern), Guha, S. (Ekstern)
Number of pages: 33
Border collisions inside the stability domain of a fixed point

Recent studies on a power electronic DC/AC converter (inverter) have demonstrated that such systems may undergo a transition from regular dynamics (associated with a globally attracting fixed point of a suitable stroboscopic map) to chaos through an irregular sequence of border-collision events. Chaotic dynamics of an inverter is not suitable for practical purposes. However, the parameter domain in which the stroboscopic map has a globally attracting fixed point has generally been considered to be uniform and suitable for practical use. In the present paper we show that this domain actually has a complicated interior structure formed by boundaries defined by persistence border collisions. We describe a simple approach that is based on symbolic dynamics and makes it possible to detect such boundaries numerically. Using this approach we describe several regions in the parameter space leading to qualitatively different output signals of the inverter although all associated with globally attracting fixed points of the corresponding stroboscopic map.

General information
State: Published
Organisations: Department of Physics, University of Stuttgart, Southwest State University
Authors: Avrutin, V. (Ekstern), Zhusubaliyev, Z. T. (Ekstern), Mosekilde, E. (Intern)
Number of pages: 15
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Publication date: 2016
Main Research Area: Technical/natural sciences

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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 1.158 SJR 0.861 CiteScore 1.75
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.847 SNIP 1.211 CiteScore 1.71
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.041 SNIP 1.29 CiteScore 1.79
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.068 SNIP 1.209 CiteScore 1.71
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.071 SNIP 1.347 CiteScore 1.76
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.083 SNIP 1.226 CiteScore 1.69
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.982 SNIP 1.165 CiteScore 1.58
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.061 SNIP 1.127
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.023 SNIP 1.164
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Bouncing droplets, pilot-waves, and quantum mechanics

Bouncing droplets on a fluid surface have recently been shown to provide a surprising analogy to quantum behaviour. Here we discuss the limitation of this analogy in the context of the double-slit experiment, which our colleagues and we have analysed in a recent paper [Phys. Rev. E 92, 013006 (2015)]. The present paper is based on the talk given by Tomas Bohr at the XX Congreso de la División de Dinámica de Fluidos, Sociedad Mexicana de Física, Centro Mesoamericana de Física Teórica, Tuxtla Gutiérrez, November 2014.

General information
State: Published
Organisations: Department of Physics, Biophysics and Fluids, University of Copenhagen
Authors: Bohr, T. (Intern), Andersen, A. P. (Intern), Lautrup, B. (Ekstern)
Number of pages: 15
Pages: 335-349
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Series: Environmental Science and Engineering
ISSN: 1863-5520
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Butterfly Deformation Modes in a Photoexcited Pyrazolate-Bridged Pt Complex Measured by Time-Resolved X-Ray Scattering in Solution

Pyrazolate-bridged dinuclear Pt(II) complexes represent a series of molecules with tunable absorption and emission properties that can be directly modulated by structural factors, such as the Pt-Pt distance. However, direct experimental information regarding the structure of the emissive triplet excited state has remained scarce. Using time-resolved wide-
angle X-ray scattering (WAXS), the excited triplet state molecular structure of [Pt(ppy)(μ-t-Bu2pz)]2 (ppy = 2-phenylpyridine; t-Bu2pz = 3,5-di-tert-butylpyrazolate), complex 1, was obtained in a dilute (0.5 mM) toluene solution utilizing the monochromatic X-ray pulses at Beamline 11IDD of the Advanced Photon Source. The excited-state structural analysis of 1 was performed based on the results from both transient WAXS measurements and density functional theory calculations to shed light on the primary structural changes in its triplet metal-metal-to-ligand charge-transfer (MMLCT) state, in particular, the Pt-Pt distance and ligand rotation. We found a pronounced Pt-Pt distance contraction accompanied by rotational motions of ppy ligands toward one another in the MMLCT state of 1. Our results suggest that the contraction is larger than what has previously been reported, but they are in good agreement with recent theoretical efforts and suggest the ppy moieties as targets for rational synthesis aimed at tuning the excited-state structure and properties.

**General information**

State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Department of Chemistry, Northwestern University, Argonne National Laboratory, North Carolina State University
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Main Research Area: Technical/natural sciences

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Volume: 120
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Ratings:
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BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 2.75
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BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.64
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
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Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 2.65
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 2.84
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 2.78
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 2.87
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Catalyst design for clean and efficient fuels

This thesis contains a theoretical approach to specific problems in catalysis and is based upon fundamental concepts from thermodynamics and density functional theory calculations. It investigates the already existing and well established process of hydrodesulfurization and a novel process of synthesizing dimethyl carbonate electrochemically. Hydrodesulfurization is an industrial refining process in which sulfur is removed from oil in order to reduce SO₂ emissions. The study on hydrodesulfurization involves determining the active sites and their atomic scale structure for the industrially used cobalt promoted MoS₂ catalyst. Reactivity of a series of model molecules, found in oil prior to desulfurization, is studied on cobalt promoted MoS₂. Such an approach has the potential to explain the underlying processes involved in the removal of sulfur at each specific site of the catalyst. The goal is to identify which sites are active towards specific molecules and in getting insight to what the ideal catalyst should look like in terms of morphology. Dimethyl carbonate is an environmentally benign compound that can be used as a solvent and precursor in chemical synthesis or as a fuel and fuel additive. It can replace different toxic compounds that are nowadays used as precursors for various reactions. An electrocatalytic process for synthesizing dimethyl carbonate is studied as part of this thesis. Producing dimethyl carbonate electrochemically makes it possible to avoid using hazardous chemical processes currently used. It is found that noble metals can be used as electrocatalysts for the synthesis of dimethyl carbonate, significantly lowering the potential when using copper instead of gold. Besides being active, copper was found to be selective towards dimethyl carbonate. A non-selective catalyst will yield unwanted coproducts, causing the need for additional separation techniques to extract pure dimethyl carbonate after synthesis. This in return increases the production cost of dimethyl carbonate.

This thesis is another step in the collective effort to make today’s fuels and chemicals environmentally friendlier and creating new, efficient and clean technologies for chemical and fuel production.

General information
State: Published
Organisations: Department of Physics, Theoretical Atomic-scale Physics
Authors: Šaric, M. (Intern), Jacobsen, K. W. (Intern), Moses, P. G. (Intern), Rossmeisl, J. (Intern)
Number of pages: 156
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Publisher: Department of Physics, Technical University of Denmark
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions: mscaric_phd_thesis_final.pdf

Relations
Projects:
Catalyst design for clean and efficient fuels
Publication: Research › Ph.D. thesis – Annual report year: 2017

Catalyst for methanol synthesis prepared by deposition precipitation

General information
State: Published
Organisations: Center for Electron Nanoscopy, DTU Danchip, Department of Physics, Experimental Surface and Nanomaterials Physics
Chemisorption of oxygen and subsequent reactions on low index surfaces of β-Mo2C: Insights from first-principles thermodynamics and kinetics

Oxygen chemisorption on β-Mo2C surfaces, the subsequent CO/CO2 desorption and oxygen diffusion to the carbon vacancy have been investigated by density-functional theory. The most stable structures together with the energetics of oxygen stepwise adsorption, CO/CO2 desorption and oxygen diffusion to the carbon vacancy were identified. We examined the effect of oxygen coverage on the morphology of β-Mo2C by plotting the equilibrium crystal shape. Thermodynamic effect of temperature and reactant or product pressure on the CO/CO2 desorption were investigated. The CO/CO2 desorption is more favorable at the saturated oxygen coverage than the low oxygen coverage thermodynamically. The subsequent oxygen diffusion to the carbon vacancy after CO/CO2 desorption may happen depending on the surfaces and oxygen coverage.
Cleaning of first mirrors in ITER by means of radio frequency discharges

First mirrors of optical diagnostics in ITER are subject to charge exchange fluxes of Be, W, and potentially other elements. This may degrade the optical performance significantly via erosion or deposition. In order to restore reflectivity, cleaning by applying radio frequency (RF) power to the mirror itself and thus creating a discharge in front of the mirror will be used. The plasma generated in front of the mirror surface sputters off deposition, restoring its reflectivity. Although the functionality of such a mirror cleaning technique is proven in laboratory experiments, the technical implementation in ITER revealed obstacles which needs to be overcome: Since the discharge as an RF load in general is not very well matched to the power generator and transmission line, power reflections will occur leading to a thermal load of the cable. Its implementation for ITER requires additional R&D. This includes the design of mirrors as RF electrodes, as well as feeders and matching networks inside the vacuum vessel. Mitigation solutions will be evaluated and discussed. Furthermore, technical obstacles (i.e., cooling water pipes for the mirrors) need to be solved. Since cooling water lines are usually on ground potential at the feed through of the vacuum vessel, a solution to decouple the ground potential from the mirror would be a major simplification. Such a solution will be presented.

General information
State: Published
Organisations: Department of Physics, Plasma Physics and Fusion Energy, ITER, RAS - Ioffe Physico Technical Institute, University of Basel
Authors: Leipold, F. (Intern), Reichle, R. (Ekstern), Vorpahl, C. (Ekstern), Mukhin, E. E. (Ekstern), Dmitriev, A. M. (Ekstern), Razdobarin, A. G. (Ekstern), Samsonov, D. S. (Ekstern), Marot, L. (Ekstern), Moser, L. (Ekstern), Steiner, R. (Ekstern), Meyer, E. (Ekstern)
Number of pages: 3
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Review of Scientific Instruments
Volume: 87
Issue number: 11
Coarsening of Pd nanoparticles in an oxidizing atmosphere studied by in situ TEM

The coarsening of supported palladium nanoparticles in an oxidizing atmosphere was studied in situ by means of transmission electron microscopy (TEM). Specifically, the Pd nanoparticles were dispersed on a planar and amorphous Al₂O₃ support and were observed during the exposure to 10 mbar technical air at 650 °C. Time-resolved TEM image series reveal that the Pd nanoparticles were immobile and that a few percent of the nanoparticles grew or shrank, indicating a coarsening process mediated by the Ostwald ripening mechanism. The TEM image contrast suggests that the largest nanoparticles tended to wet the Al₂O₃ support to a higher degree than the smaller nanoparticles and that the distribution of projected particle sizes consequently broadens by the appearance of an asymmetric tail toward the larger particle sizes. A comparison with computer simulations based on a simple mean-field model for the Ostwald ripening process indicates that the observed change in the particle size distribution can be accounted for by wetting of the Al₂O₃ support by the larger Pd nanoparticles.

General information
State: Published
Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics, Center for Individual Nanoparticle Functionality, Haldor Topsoe AS, Chalmers University of Technology
Authors: Simonsen, S. B. (Intern), Chorkendorff, I. (Intern), Dahl, S. (Ekstern), Skoglundh, M. (Ekstern), Helveg, S. (Ekstern)
Number of pages: 6
Pages: 278-283
Publication date: 2016
Main Research Area: Technical/natural sciences

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Journal: Surface Science
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Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 0.759 SJR 0.81 CiteScore 1.87
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.85 SJR 0.746 SNIP 0.834
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.747 SNIP 0.804 CiteScore 1.85
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.818 SNIP 0.864 CiteScore 1.81
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.829 SNIP 0.781 CiteScore 1.72
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.096 SNIP 0.878 CiteScore 1.91
ISI indexed (2012): ISI indexed yes
Cold pulse and rotation reversals with turbulence spreading and residual stress
Transport modeling based on inclusion of turbulence spreading and residual stresses shows internal rotation reversals and polarity reversal of cold pulses, with a clear indication of nonlocal transport effects due to fast spreading in the turbulence intensity field. The effects of turbulence spreading and residual stress are calculated from the gradient of the turbulence intensity. In the model presented in this paper, the flux is carried by the turbulence intensity field, which in itself is subject to radial transport effects. The pulse polarity inversion and the rotation profile reversal positions are close to the radial location of the stable/unstable transition. Both effects have no direct explanation within the framework of classical transport modeling, where the fluxes are related directly to the linear growth rates, the turbulence intensity profile is not considered and the corresponding residual stress is absent. Our simulations are in qualitative agreement with measurements from ohmically heated plasmas. Rotation reversal at a finite radius is found in situations not displaying saturated confinement, which we identify as situations where the plasma is nearly everywhere unstable. As an additional and new effect, the model predicts a perturbation of the velocity profile following a cold pulse from the edge. This allows direct experimental confirmation of both the existence of residual stress caused by turbulence intensity profiles and fundamental ideas of transport modeling presented here. Published by AIP Publishing.
Cold pulse and rotation reversals with turbulence spreading and residual stress

General information
State: Published
Authors: Hariri, F. (Ekstern), Naulin, V. (Intern), Rasmussen, J. J. (Intern)
Number of pages: 1
Publication date: 2016
Main Research Area: Technical/natural sciences

Collective Thomson scattering measurements of fast-ion transport due to sawtooth crashes in ASDEX Upgrade

Sawtooth instabilities can modify heating and current-drive profiles and potentially increase fast-ion losses. Understanding how sawteeth redistribute fast ions as a function of sawtooth parameters and of fast-ion energy and pitch is hence a subject of particular interest for future fusion devices. Here we present the first collective Thomson scattering (CTS) measurements of sawtooth-induced redistribution of fast ions at ASDEX Upgrade. These also represent the first localized fast-ion measurements on the high-field side of this device. The results indicate fast-ion losses in the phase-space measurement volume of about 50% across sawtooth crashes, in good agreement with values predicted with the Kadomtsev sawtooth model implemented in TRANSP and with the sawtooth model in the EBdyna_go code. In contrast to the case of sawteeth, we observe no fast-ion redistribution in the presence of fishbone modes. We highlight how CTS measurements can discriminate between different sawtooth models, in particular when aided by multi-diagnostic velocity-space tomography, and briefly discuss our results in light of existing measurements from other fast-ion diagnostics.

General information
State: Published
Organisations: Department of Physics, Plasma Physics and Fusion Energy, University of Seville, Max-Planck-Institut fur Plasmaphysik, FOM Dutch Institute for Fundamental Energy Research, Budapest University of Technology and Economics
Number of pages: 9
Pages: 112014
Publication date: 2016
Main Research Area: Technical/natural sciences
Fast ions in tokamaks, Collective Thomson scattering, Fast-ion velocity distribution function, Sawtooth instabilities
Collisional transport across the magnetic field in drift-fluid models
Drift ordered fluid models are widely applied in studies of low-frequency turbulence in the edge and scrape-off layer regions of magnetically confined plasmas. Here, we show how collisional transport across the magnetic field is self-consistently incorporated into drift-fluid models without altering the drift-fluid energy integral. We demonstrate that the inclusion of collisional transport in drift-fluid models gives rise to diffusion of particle density, momentum, and pressures in drift-fluid turbulence models and, thereby, obviates the customary use of artificial diffusion in turbulence simulations. We further derive a computationally efficient, two-dimensional model, which can be time integrated for several turbulence decorrelation times using only limited computational resources. The model describes interchange turbulence in a two-dimensional plane perpendicular to the magnetic field located at the outboard midplane of a tokamak. The model domain has two regions modeling open and closed field lines. The model employs a computational expedient model for collisional transport. Numerical simulations show good agreement between the full and the simplified model for collisional transport.

General information
State: Published
Organisations: Department of Physics, Plasma Physics and Fusion Energy
Authors: Madsen, J. (Intern), Naulin, V. (Intern), Nielsen, A. H. (Intern), Rasmussen, J. J. (Intern)
Number of pages: 14
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Main Research Area: Technical/natural sciences

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Journal: Physics of Plasmas
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Article number: 032306
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BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
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Scopus rating (2017): SNIP 0.682 SJR 0.576 CiteScore 1.17
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.08 SJR 0.999 SNIP 1.052
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.874 SNIP 0.908 CiteScore 1.02
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.153 SNIP 1.195 CiteScore 1.69
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.114 SNIP 1.224 CiteScore 1.7
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.439 SNIP 1.255 CiteScore 1.83
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.221 SNIP 1.27 CiteScore 2.09
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
Combining X-ray and Electron Based in situ Characterization of Catalysts

General information
State: Published
Organisations: Center for Electron Nanoscopy, Department of Physics, Experimental Surface and Nanomaterials Physics
Authors: Damsgaard, C. D. (Intern)
Publication date: 2016
Event: Abstract from 3rd International Conference on In-Situ and Correlative Electron Microscopy, Saarbrücken, Germany.
Main Research Area: Technical/natural sciences
Electronic versions: CISCEM_2016_cdda_final_2.pdf
Source: PublicationPreSubmission
Source-ID: 127046032
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2016

Comparison of Pulsed Electron Deposition and Pulsed Laser Deposition of selected materials

General information
State: Published
Organisations: Department of Photonics Engineering, Department of Micro- and Nanotechnology, Experimental Surface and Nanomaterials Physics, Silicon Microtechnology, Photovoltaic Materials and Systems, Consiglio Nazionale delle Ricerche, Technical University of Denmark
Authors: Ettlinger, R. B. (Intern), Pattini, F. (Ekstern), Rampino, S. (Ekstern), Cazzaniga, A. C. (Intern), Crovetto, A. (Intern), Bosco, E. (Ekstern), Gilioli, E. (Ekstern), Hansen, O. (Intern), Schou, J. (Intern)
Composition-dependent variation of magnetic properties and interstitial ordering in homogeneous expanded austenite

The crystal structure and magnetic properties of austenitic stainless steel with a colossal interstitial content, so-called expanded austenite, are currently not completely understood. In the present work, the magnetic properties of homogeneous samples of expanded austenite, as prepared by low-temperature nitriding of thin foils, were investigated with magnetometry and Mössbauer spectroscopy. At room temperature, expanded austenite is paramagnetic for relatively low and for relatively high nitrogen contents ($y_N = 0.13$ and $0.55$, respectively, where $y_N$ is the interstitial nitrogen occupancy), while ferromagnetism is observed for intermediate nitrogen loads. Spontaneous volume magnetostriction was observed in the ferromagnetic state and the Curie temperature was found to depend strongly on the nitrogen content. For the first time, X-ray diffraction evidence for the occurrence of long-range interstitial order of nitrogen atoms in expanded austenite was observed for high nitrogen contents.
Compound waves in a higher order nonlinear model of thermoviscous fluids

A generalized traveling wave ansatz is used to investigate compound shock waves in a higher order nonlinear model of a thermoviscous fluid. The fluid velocity potential is written as a traveling wave plus a linear function of space and time. The latter offers the possibility of predicting the outcome of interacting shock waves, i.e., shock jump heights and wave velocities after collisions and overtakes. The stability of the linear solution part is investigated and a criterion for its stability is determined. For a number of instances, the numerical results show formation of rarefaction waves. By using a similarity transformation, analytical expressions for these rarefaction waves are found in the limit of no dissipation. Examples of compound shock waves are illustrated by numerical simulations.
Continuous-variable quantum computing on encrypted data

The ability to perform computations on encrypted data is a powerful tool for protecting a client's privacy, especially in today's era of cloud and distributed computing. In terms of privacy, the best solutions that classical techniques can achieve are unfortunately not unconditionally secure in the sense that they are dependent on a hacker's computational power. Here we theoretically investigate, and experimentally demonstrate with Gaussian displacement and squeezing operations, a quantum solution that achieves the security of a user's privacy using the practical technology of continuous variables. We demonstrate losses of up to 10 km both ways between the client and the server and show that security can still be achieved. Our approach offers a number of practical benefits (from a quantum perspective) that could one day allow the potential widespread adoption of this quantum technology in future cloud-based computing networks.

General information

State: Published
Organisations: Department of Physics, Quantum Physics and Information Technology, University of Toronto, CipherQ
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Main Research Area: Technical/natural sciences

Publication information

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Article number: 13795
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- Web of Science (2018): Indexed yes
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- Scopus rating (2017): CiteScore 12.41 SJR 6.582 SNIP 2.912
- Web of Science (2017): Indexed yes
- BFI (2016): BFI-level 2
- Scopus rating (2016): CiteScore 11.8 SJR 6.414 SNIP 2.855
- Web of Science (2016): Indexed yes
- BFI (2015): BFI-level 1
- Scopus rating (2015): SJR 6.287 SNIP 2.86 CiteScore 11.23
- Web of Science (2015): Indexed yes
- BFI (2014): BFI-level 1
- Scopus rating (2014): SJR 6.41 SNIP 3.034 CiteScore 10.77
- Web of Science (2014): Indexed yes
- BFI (2013): BFI-level 1
- Scopus rating (2013): SJR 6.206 SNIP 2.797 CiteScore 9.85
- ISI indexed (2013): ISI indexed yes
- Web of Science (2013): Indexed yes
- Scopus rating (2012): SJR 5.866 SNIP 2.829 CiteScore 8.32
- ISI indexed (2012): ISI indexed yes
- Web of Science (2012): Indexed yes
- Scopus rating (2011): SJR 3.137 SNIP 1.825 CiteScore 4.44
- ISI indexed (2011): ISI indexed no
- Web of Science (2010): Indexed yes
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Continuum modeling of hydrodynamic particle–particle interactions in microfluidic high-concentration suspensions

A continuum model is established for numerical studies of hydrodynamic particle–particle interactions in microfluidic high-concentration suspensions. A suspension of microparticles placed in a microfluidic channel and influenced by an external force, is described by a continuous particle-concentration field coupled to the continuity and Navier–Stokes equation for the solution. The hydrodynamic interactions are accounted for through the concentration dependence of the suspension viscosity, of the single-particle mobility, and of the momentum transfer from the particles to the suspension. The model is applied on a magnetophoretic and an acoustophoretic system, respectively, and based on the results, we illustrate three main points: (1) for relative particle-to-fluid volume fractions greater than 0.01, the hydrodynamic interaction effects become important through a decreased particle mobility and an increased suspension viscosity. (2) At these high particle concentrations, particle-induced flow rolls occur, which can lead to significant deviations of the advective particle transport relative to that of dilute suspensions. (3) Which interaction mechanism that dominates, depends on the specific flow geometry and the specific external force acting on the particles.
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.673 SNIP 2.164
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 2.833 SNIP 1.849
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 2.441 SNIP 1.827
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 2.564 SNIP 1.61
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.52 SNIP 1.428
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.962 SNIP 1.823
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.126 SNIP 1.466
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 1.28 SNIP 0.904
Web of Science (2002): Indexed yes
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This is a correction to the manuscript.

**General information**
State: Published
Organisations: Department of Physics, Quantum Physics and Information Techology
Authors: Jacobsen, C. S. (Intern), Gehring, T. (Intern), Andersen, U. L. (Intern)
Publication date: 2016
Main Research Area: Technical/natural sciences

**Publication information**
Journal: Entropy
ISSN (Print): 1099-4300
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 1.189 SJR 0.592 CiteScore 2.41
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.87 SJR 0.56 SNIP 1.109
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.551 SNIP 1.14 CiteScore 1.99
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Correlated classical states outperform squeezed states in communication over Gaussian channels

Using a quantum amplifier in a Gaussian channel, we show that classically correlated input states can outperform the mutual information of squeezed states.

General information
State: Published
Organisations: Department of Physics, Quantum Physics and Information Technology
Authors: Schäfermeier, C. (Intern), Andersen, U. L. (Intern)
Number of pages: 2
Pages: 1-2
Publication date: 2016

Host publication information
Title of host publication: 2016 Conference on Lasers and Electro-optics
Publisher: IEEE
ISBN (Print): 978-1-5090-2434-6
Main Research Area: Technical/natural sciences
Conference: Conference on Lasers and Electro-Optics 2016, San Jose, California, United States, 05/06/2016 - 05/06/2016
Source: FindIt
Source-ID: 2350003243
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2016
Correlation between diffusion barriers and alloying energy in binary alloys

In this paper, we explore the notion that a negative alloying energy may act as a descriptor for long term stability of Pt-alloys as cathode catalysts in low temperature fuel cells.

General information
State: Published
Organisations: Experimental Surface and Nanomaterials Physics, Department of Physics
Authors: Vej-Hansen, U. G. (Intern), Rossmeisl, J. (Intern), Stephens, I. (Intern), Schiøtz, J. (Intern)
Number of pages: 6
Pages: 3302-3307
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Physical Chemistry Chemical Physics
Volume: 18
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ISSN (Print): 1463-9076
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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
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
Coupling single emitters to quantum plasmonic circuits

In recent years, the controlled coupling of single-photon emitters to propagating surface plasmons has been intensely studied, which is fueled by the prospect of a giant photonic nonlinearity on a nanoscaled platform. In this article, we will review the recent progress on coupling single emitters to nanowires towards the construction of a new platform for strong light-matter interaction. The control over such a platform might open new doors for quantum information processing and quantum sensing at the nanoscale and for the study of fundamental physics in the ultrastrong coupling regime.

General information
State: Published
Organisations: Department of Physics, Quantum Physics and Information Technology
Authors: Huck, A. (Intern), Andersen, U. L. (Intern)
Number of pages: 13
Pages: 483-495
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Nanophotonics
Volume: 5
Issue number: 3
ISSN (Print): 2192-8606
Ratings:
Web of Science (2018): Indexed yes
Scopus rating (2017): CiteScore 6.57 SJR 2.916 SNIP 1.892
Deactivation of Ni-MoS2 by bio-oil impurities during hydrodeoxygenation of phenol and octanol

The stability of Ni-MoS2/ZrO2 toward water, potassium, and chlorine containing compounds during hydrodeoxygenation (HDO) of a mixture of phenol and 1-octanol was investigated in a high pressure gas and liquid continuous flow fixed bed setup at 280 °C and 100 bar. To maintain the stability of the catalyst, sufficient co-feeding of a sulfur source was necessary to avoid oxidation of the sulfide phase by oxygen replacement of the edge sulfur atoms in the MoS2 structure. However, the addition of sulfur to the feed gas resulted in the formation of sulfur containing compounds, mainly thiols, in the oil product if the residence time was too low. At a weight hourly space velocity (WHSV) of 4.9 h⁻¹ the sulfur content in the liquid product was 980 ppm by weight, but this could be decreased to 5 ppm at a WHSV of 1.4 h⁻¹. A high co-feed of sulfur was needed when water was present in the feed and the H2O/H2S molar ratio should be below ca. 10 to maintain a decent stability of the catalyst. Chlorine containing compounds caused a reversible deactivation of the catalyst when co-fed to the reactor, where the catalytic activity could be completely regained when removing it from the feed. Commonly, chlorine, H2O, and H2S all inhibited the activity of the catalyst by competing for the active sites, with chlorine being by far the strongest inhibitor and H2S and H2O of roughly the same strength. Dissimilar, potassium was a severe poison and irreversibly deactivated the catalyst to <5% degree of deoxygenation when impregnated on the catalyst in a stoichiometric ratio relative to the active metal. This deactivation was a result of adsorption of potassium on the edge vacancy sites of the MoS2 slabs.
Defect-Tolerant Monolayer Transition Metal Dichalcogenides

Localized electronic states formed inside the band gap of a semiconductor due to crystal defects can be detrimental to the material's optoelectronic properties. Semiconductors with a lower tendency to form defect induced deep gap states are termed defect-tolerant. Here we provide a systematic first-principles investigation of defect tolerance in 29 monolayer transition metal dichalcogenides (TMDs) of interest for nanoscale optoelectronics. We find that the TMDs based on group VI and X metals form deep gap states upon creation of a chalcogen (S, Se, Te) vacancy, while the TMDs based on group IV metals form only shallow defect levels and are thus predicted to be defect-tolerant. Interestingly, all the defect sensitive TMDs have valence and conduction bands with a very similar orbital composition. This indicates a bonding/antibonding nature of the gap, which in turn suggests that dangling bonds will fall inside the gap. These ideas are made quantitative by introducing a descriptor that measures the degree of similarity of the conduction and valence band manifolds. Finally, the study is generalized to nonpolar nanoribbons of the TMDs where we find that only the defect sensitive materials form edge states within the band gap.
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
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Original language: English
2D materials, Defect tolerance, Density functional theory, Descriptor, Fingerprint, Nanoribbon
DOIs:
10.1021/acs.nanolett.5b04513
Links:
https://arxiv.org/abs/1604.03232
Source: FindIt
Source-ID: 2303177353
Publication: Research - peer-review › Journal article – Annual report year: 2016

Depth-dependent composition of sputtered ZnO:Al

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, Experimental Surface and Nanomaterials Physics, Technical University of Denmark
Authors: Crovetto, A. (Intern), Ottsen, T. (Ekstern), Stamate, E. (Intern), Kjær, D. (Intern), Schou, J. (Intern), Hansen, O. (Intern)
Number of pages: 1
Publication date: 2016
Event: Poster session presented at 6th International Symposium on Transparent Conductive Materials, Chania, Greece.
Main Research Area: Technical/natural sciences
Electronic versions:
Andrea_Poster_TCM2016_final.pdf
Source: PublicationPreSubmission
Source-ID: 126934871
Publication: Research - peer-review › Poster – Annual report year: 2016

Designing in-plane heterostructures of quantum spin Hall insulators from first principles: 1T'-MoS2 with adsorbates
Interfaces between normal and topological insulators are bound to host metallic states that are protected by time-reversal symmetry and are therefore robust against disorder and interface reconstruction. Two-dimensional topological insulators (quantum spin Hall insulators) offer a unique opportunity to change the local topology by adsorption of atoms or molecules and thus comprise an ideal platform for designing topological heterostructures. Here we apply first-principles calculations to show that the quantum spin Hall insulator 1T'-MoS2 exhibits a phase transition to a trivial insulator upon adsorption of various atoms. It is then demonstrated that one-dimensional metallic states indeed arise at the boundary of regions with and without adsorbed oxygen and that these boundary states generically constitute simple linear connections between valence and conduction bands in reciprocal space. This is in sharp contrast to topological edge states, which typically exhibit strong dispersion that are sensitive to a particular edge termination. The heterostructure is also suggestive of a simple design of one-dimensional metallic networks in sheets of 1T'-MoS2.

General information
State: Published
Organisations: Department of Physics, Theoretical Atomic-scale Physics, Center for Nanostructured Graphene
Design of the Collective Thomson Scattering diagnostic for the next-generation fusion experiment ITER

General information
State: Published
Organisations: Department of Physics, Plasma Physics and Fusion Energy, Center for Nuclear Technologies, Radiation Physics, Universidade de Lisboa, Fusion For Energy
Publication date: 2016
Event: Abstract from Dansk Fysisk Selskab Årsmøde 2016, Middelfart, Denmark.
Main Research Area: Technical/natural sciences

Determining the internal quantum efficiency of shallow-implanted nitrogen-vacancy defects in bulk diamond

It is generally accepted that nitrogen-vacancy (NV) defects in bulk diamond are bright sources of luminescence. However, the exact value of their internal quantum efficiency (IQE) has not been measured so far. Here we use an implementation of Drexhage’s scheme to quantify the IQE of shallow-implanted NV defects in a single-crystal bulk diamond. Using a spherical metallic mirror with a large radius of curvature compared to the optical spot size, we perform calibrated modifications of the local density of states around NV defects and observe the change of their total decay rate, which is further used for IQE quantification. We also show that at the excitation wavelength of 532 nm, photo-induced relaxation cannot be neglected even at moderate excitation powers well below the saturation level. For NV defects shallow implanted 4.5 ± 1 and 8 ± 2 nm below the diamond surface, we determine the quantum efficiency to be 0.70 ± 0.07 and 0.82 ± 0.08, respectively.

General information
State: Published
Organisations: Department of Physics, Quantum Physics and Information Technology, Department of Photonics Engineering, Fiber Sensors and Supercontinuum Generation, University of Leipzig, University of Ulm
Authors: Radko, I. (Intern), Bolt, M. (Intern), Israelsen, N. M. (Intern), Raatz, N. (Ekstern), Meijer, J. (Ekstern), Jelezko, F. (Ekstern), Andersen, U. L. (Intern), Huck, A. (Intern)
Number of pages: 11
Pages: 27715-27725
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Optics Express
Volume: 24
Issue number: 24
ISSN (Print): 1094-4087
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): SJR 1.519 SNIP 1.567 CiteScore 3.74
Developing diagnostic systems for ITER – the next step fusion energy experiment

Fusion energy research is moving to the next stage with the well progressed construction of one of the largest research infrastructures ever – ITER. The goal of ITER is to produce 500 MW of fusion power while heating the fuel – deuterium/tritium plasma – by 50 MW. This will confirm fusion energy to be a viable energy source. Fusion energy power plants will be safe and can be operated to supply the baseload of an energy system. The fuel resources are inexhaustible, and can be derived from sea water. Fusion energy is based on the nuclear reaction fusing hydrogen isotopes into helium – like in the Sun – and thus no CO2 is released in the energy production. The waste of the energy production is the irradiated steel of the core of the reactor, but this radioactivity will only last for about 100 years and no long-term radioactive waste storage is needed.

While the promise of safe, clean and abundant energy is the ultimate goal of fusion energy, the path towards this is challenging. A fusion plasma has a temperature of 200 mio. degrees (15 times that of the core of the Sun), and this is confined by a magnetic field generated by powerful superconducting magnets in a vacuum chamber of 1000 m³. Operating diagnostic systems in the environment of ITER is a challenge for many technologies, but due to robustness, microwave diagnostics will play an increasingly important role in burning plasma fusion energy experiments like ITER and beyond. The Collective Thomson Scattering (CTS) diagnostic to be installed at ITER is an example of such a diagnostic with great potential in present and future experiments. The ITER CTS diagnostic will inject a 1 MW 60 GHz beam of electromagnetic radiation from a gyrotron into the ITER plasma and observe the scattering off fluctuations in the plasma – to monitor the dynamics of the fast ions generated in the fusion reactions. This will provide important physics understanding of the behavior of the fusion plasma that can be used for optimizing future fusion power plants. A research team at DTU (DTU Physics and DTU Nutech) has been tasked by Fusion for Energy (the European coordinator for supplies to ITER) to develop the ITER CTS diagnostic in collaboration with Instituto Superior Técnico in Portugal. It is a 5 year effort of more than 50 man year total effort. This presentation will outline the prospects and the status of the development of fusion energy research and the CTS diagnostic system for ITER.

Development of a synthetic lithium beam diagnostic for the HESEL turbulence code and application to blob transport

The synthetic Li-BES system included in the first principle model HESEL shows, that it can be used for quantitative analysis of blob characteristics. It is suitable to be compared to experimental Li-BES results. The results of the radial analysis affirm, that the synthetic Li-BES measurements deliver reliable blob velocities. The velocity scaling investigations show a good agreement with the scaling laws, but need to be corrected for a true representation.
Dielectric function and double absorption onset of monoclinic Cu$_2$SnS$_3$: Origin of experimental features explained by first-principles calculations

In this work, we determine experimentally the dielectric function of monoclinic Cu$_2$SnS$_3$ (CTS) by spectroscopic ellipsometry from 0.7 to 5.9 eV. An experimental approach is proposed to overcome the challenges of extracting the dielectric function of Cu$_2$SnS$_3$ when grown on a glass/Mo substrate, as relevant for photovoltaic applications. The ellipsometry measurement reveals a double absorption onset at 0.91 eV and 0.99 eV. Importantly, we demonstrate that calculation within the density functional theory (DFT) confirms this double onset only when a very dense k-mesh is used to reveal fine details in the electronic structure, and this can explain why it has not been reported in earlier calculated spectra. We can now show that the double onset originates from optical transitions at the Γ-point from three energetically close-lying valence bands to a single conduction band. Thus, structural imperfection, like secondary phases, is not needed to explain such an absorption spectrum. Finally, we show that the absorption coefficient of CTS is particularly large in the near-band gap spectral region when compared to similar photovoltaic materials.

General information

State: Published
Organisations: Department of Micro- and Nanotechnology, Silicon Microtechnology, Department of Photonics Engineering, Optical Microsensors and Micromaterials, Experimental Surface and Nanomaterials Physics, KTH - Royal Institute of Technology, University of Oslo
Authors: Crovetto, A. (Intern), Chen, R. (Ekstern), Ettlinger, R. B. (Intern), Cazzaniga, A. C. (Intern), Schou, J. (Intern), Persson, C. (Ekstern), Hansen, O. (Intern)
Pages: 121-129
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information

Volume: 154
ISSN (Print): 0927-0248
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): SNIP 1.532 SJR 1.459 CiteScore 4.83
BFI (2016): BFI-level 2
Web of Science (2016): Indexed yes
Scopus rating (2016): CiteScore 4.97 SJR 1.599 SNIP 1.71
BFI (2015): BFI-level 2
Web of Science (2015): Indexed yes
Scopus rating (2015): SJR 1.8 SNIP 1.851 CiteScore 5.16
BFI (2014): BFI-level 2
Web of Science (2014): Indexed yes
Scopus rating (2014): SJR 2.19 SNIP 2.348 CiteScore 5.87
Web of Science (2013): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 2.179 SNIP 2.529 CiteScore 5.58
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.441 SNIP 2.654 CiteScore 5.25
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Direct observation of grain rotations during coarsening of a semisolid Al-Cu alloy

Sintering is a key technology for processing ceramic and metallic powders into solid objects of complex geometry, particularly in the burgeoning field of energy storage materials. The modeling of sintering processes, however, has not kept pace with applications. Conventional models, which assume ideal arrangements of constituent powders while ignoring their underlying crystallinity, achieve at best a qualitative description of the rearrangement, densification, and coarsening of powder compacts during thermal processing. Treating a semisolid Al-Cu alloy as a model system for late-stage sintering—during which densification plays a subordinate role to coarsening—we have used 3D X-ray diffraction microscopy to track the changes in sample microstructure induced by annealing. The results establish the occurrence of significant particle rotations, driven in part by the dependence of boundary energy on crystallographic misorientation. Evidently, a comprehensive model for sintering must incorporate crystallographic parameters into the thermodynamic driving forces governing microstructural evolution.

General information

State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, University of Ulm, University of Copenhagen, Japan Synchrotron Radiation Research Institute
Authors: Dake, J. M. (Ekstern), Oddershede, J. (Intern), Sørensen, H. O. (Ekstern), Werz, T. (Ekstern), Shatto, J. C. (Ekstern), Uesugi, K. (Ekstern), Schmidt, S. (Intern), Krill III, C. E. (Ekstern)
Number of pages: 9
Pages: E5998 – E6006
Publication date: 2016
Main Research Area: Technical/natural sciences
Direct observation of the thermal demagnetization of magnetic vortex structures in nonideal magnetite recorders: Thermal Demagnetization of Vortex States

The thermal demagnetization of pseudo-single-domain (PSD) magnetite ($\text{Fe}_3\text{O}_4$) particles, which govern the magnetic signal in many igneous rocks, is examined using off-axis electron holography. Visualization of a vortex structure held by an individual $\text{Fe}_3\text{O}_4$ particle (~250nm in diameter) during in situ heating is achieved through the construction and examination of magnetic-induction maps. Stepwise demagnetization of the remanence-induced $\text{Fe}_3\text{O}_4$ particle upon heating to above the Curie temperature, performed in a similar fashion to bulk thermal demagnetization measurements, revealed that its vortex state remains stable under heating close to its unblocking temperature and is recovered upon cooling with the same or reversed vorticity. Hence, the PSD Fe3O4 particle exhibits thermomagnetic behavior comparable to a single-domain carrier, and thus, vortex states are considered reliable magnetic recorders for paleomagnetic investigations.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Imperial College London, University of Edinburgh, Research Centre Julich (FZJ)
Authors: Almeida, T. P. (Ekstern), Muxworthy, A. R. (Ekstern), Kovács, A. (Ekstern), Williams, W. (Ekstern), Nagy, L. (Ekstern), Conbhui, P. O. (Ekstern), Frandsen, C. (Intern), Supakulopas, R. (Ekstern), Dunin-Borkowski, R. E. (Ekstern)
Number of pages: 9
Pages: 8426-8434
Publication date: 2016
Main Research Area: Technical/natural sciences
Publication information
Journal: Geophysical Research Letters
Volume: 43
Issue number: 16
ISSN (Print): 0094-8276
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 4.51 SJR 2.657 SNIP 1.429
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.35 SJR 2.819 SNIP 1.495
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 3.144 SNIP 1.496 CiteScore 4.27
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 3.135 SNIP 1.552 CiteScore 4.26
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 3.24 SNIP 1.728 CiteScore 4.45
ISI indexed (2013): ISI indexed yes
Electrochemical reactions play an increasingly important role in sustainable energy conversion and chemical synthesis. Better understanding of catalytic mechanisms at electrode surfaces is thus important for the transition to a clean-energy economy, but is hindered by the difficulty of real-time detection of products and reaction intermediates during electrochemistry experiments. Electrochemical mass spectrometry (EC-MS), including techniques referred to as DEMS and OLEMS, can enable in-situ detection of electrochemical products, but often fails to provide quantitative or reproducible results.

Herein, we present a new type of EC-MS based on a versatile gas inlet to vacuum fabricated onto a silicon microchip, and compare it to established techniques with focus on sensitivity, time response, and mass transport. The chip consists of a
perforated membrane stabilizing a large liquid-gas interface, a capillary maintaining a controlled flow over a pressure drop to ultra-high vacuum, and inlet and outlet channels for an inert make up gas. The use of a direct inlet enables orders of magnitude higher sensitivity than differentially pumped systems without a loss in time response for volatile products, while clean-room techniques for chipfabrication and a precisely controlled working distance between the electrode and chip membrane provide for a highly reproducible experimental setup. The make up gas can also be used to saturate the electrolyte from through the chip membrane enabling quick and precise exchange of dissolved gases. The well-characterized mass transport of both reactants and products in this setup enables single-turnover resolution for analysis of electrochemical reactions, as will be demonstrated with examples.

General information
State: Published
Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics, Department of Micro- and Nanotechnology, Silicon Microtechnology
Number of pages: 1
Publication date: 2016
Main Research Area: Technical/natural sciences
Links:
http://www.sustain.dtu.dk/

Bibliographical note
Sustain Abstract U-8
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2016

Disrupted bandcount doubling in an AC-DC boost PFC circuit modeled by a time varying map
Power factor correction converters are used in many applications as AC-DC power supplies aiming at maintaining a near unity power factor. Systems of this type are known to exhibit nonlinear phenomena such as sub-harmonic oscillations and chaotic regimes that cannot be described by traditional averaged models. In this paper, we derive a time varying discretetime map modeling the behavior of a power factor correction AC-DC boost converter. This map is derived in closed-form and is able to faithfully reproduce the system behavior under realistic conditions. In the chaotic regime the map exhibits a sequence of bifurcation similar to a bandcount doubling cascade on the low frequency. However, the observed scenario appears in some sense incomplete, with some gaps in the bifurcation diagram, whose appearance to our knowledge has never been reported before. We show that these gaps are caused by high frequency oscillations.

General information
State: Published
Organisations: Department of Physics, Southwest State University, University of Stuttgart, Universitat Rovira i Virgili, Universite de Toulouse
Number of pages: 13
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Physics: Conference Series
Volume: 692
Issue number: 1
Article number: 012003
ISSN (Print): 1742-6596
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 0.48 SJR 0.241 SNIP 0.447
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 0.45 SJR 0.24 SNIP 0.401
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Dual strain mechanisms in a lead-free morphotropic phase boundary ferroelectric

Electromechanical properties such as $d_{33}$ and strain are significantly enhanced at morphotropic phase boundaries (MPBs) between two or more different crystal structures. Many actuators, sensors and MEMS devices are therefore systems with MPBs, usually between polar phases in lead (Pb)-based ferroelectric ceramics. In the search for Pb-free alternatives, systems with MPBs between polar and non-polar phases have recently been theorized as having great promise. While such an MPB was identified in rare-earth (RE) modified bismuth ferrite (BFO) thin films, synthesis challenges have prevented its realization in ceramics. Overcoming these, we demonstrate a comparable electromechanical response to Pb-based materials at the polar-to-non-polar MPB in Sm modified BFO. This arises from 'dual' strain mechanisms: ferroelectric/ferroelastic switching and a previously unreported electric-field induced transition of an anti-polar intermediate phase. We show that intermediate phases play an important role in the macroscopic strain response, and may have potential to enhance electromechanical properties at polar-to-non-polar MPBs.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Josef Stefan Institute, Ural Federal University, University of New South Wales
Authors: Walker, J. (Ekstern), Simons, H. (Intern), Alikin, D. O. (Ekstern), Turygin, A. P. (Ekstern), Shur, V. Y. (Ekstern), Kholkin, A. L. (Ekstern), Ursic, H. (Ekstern), Bencan, A. (Ekstern), Malic, B. (Ekstern), Nagarajan, V. (Ekstern), Rojac, T. (Ekstern)
Number of pages: 8
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Scientific Reports
Volume: 6
Article number: 19630
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:
srep19630.pdf
DOIs:
10.1038/srep19630

Bibliographical note
Dynamic reaction phenomena during electrochemical reduction of CO on size selected copper nanoparticles

General information
State: Published
Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics
Authors: Scott, S. B. (Intern), Trimarco, D. B. (Intern), Chorkendorff, I. (Intern)
Number of pages: 1
Publication date: 2016
Main Research Area: Technical/natural sciences
Links:
http://www.sustain.dtu.dk/

Bibliographical note
Sustain Abstract E-19
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2016

Effect of side-chain asymmetry on the intermolecular structure and order-disorder transition in alkyl-substituted polyfluorenes
We study relations among the side-chain asymmetry, structure, and order-disorder transition (ODT) in hairy-rod-type poly(9,9-dihexylfluorene) (PF6) with two identical side chains and atactic poly(9-octyl-9-methyl-fluorene) (PF1-8) with two different side chains per repeat. PF6 and PF1-8 organize into alternating side-chain and backbone layers that transform into an isotropic phase at TODT (PF6) and TODT (PF1-8). We interpret polymers in terms of monodisperse and bidisperse brushes and predict scenarios TODT < TODT (PF1-8) for high and low grafting densities (the side-chain length above or below the average grafting distance). Calorimetry and x-ray scattering indicate the condition TODT (PF6) ≈ TODT (PF1-8) following the low grafting prediction. PF6 side chains coming from the alternating backbone layers appear as two separate layers with thickness H(PF6), whereas PF1-8 side chains appear as an indistinguishable bilayer with a half thickness Hbilayer(PF1-8)/2 ≈ H(PF6). The low grafting density region is structurally possible but not certain for PF6 and confirmed for PF1-8.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, DSM Research, University of Helsinki, Lund University, Bergische Universität Wuppertal
Authors: Knaapila, M. (Intern), Stepanyan, R. (Ekstern), Torkkeli, M. (Ekstern), Haase, D. (Ekstern), Fröhlich, N. (Ekstern), Helfer, A. (Ekstern), Forster, M. (Ekstern), Scherf, U. (Ekstern)
Number of pages: 8
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Physical Review E
Volume: 93
Issue number: 4
Article number: 042504
ISSN (Print): 2470-0045
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 0.987 SJR 0.979 CiteScore 2.14
Web of Science (2017): Indexed Yes
Scopus rating (2016): CiteScore 1.95 SJR 1.271 SNIP 1.018
Web of Science (2016): Indexed yes
Scopus rating (2015): SJR 1.183 SNIP 1.043 CiteScore 1.89
Web of Science (2015): Indexed yes
Scopus rating (2014): SJR 1.244 SNIP 1.135 CiteScore 2.05
Efficient generation of 1.9 W yellow light by cascaded frequency doubling of a distributed Bragg reflector tapered diode

Watt-level yellow emitting lasers are interesting for medical applications, due to their high hemoglobin absorption, and for efficient detection of certain fluorophores. In this paper, we demonstrate a compact and robust diode-based laser system in the yellow spectral range. The system generates 1.9 W of single-frequency light at 562.4 nm by cascaded single-pass frequency doubling of the 1124.8 nm emission from a distributed Bragg reflector (DBR) tapered laser diode. The absence of a free-space cavity makes the system stable over a base-plate temperature range of 30 K. At the same time, the use of a laser diode enables the modulation of the pump wavelength by controlling the drive current. This is utilized to achieve a power modulation depth above 90% for the second harmonic light, with a rise time below 40 μs.

General information
State: Published
Organisations: Department of Photonics Engineering, Diode Lasers and LED Systems, Department of Applied Mathematics and Computer Science, Department of Physics, Others, Risø National Laboratory for Sustainable Energy,
Efficient many-body calculations for two-dimensional materials using exact limits for the screened potential: Band gaps of MoS$_2$, h-BN, and phosphorene

Calculating the quasiparticle (QP) band structure of two-dimensional (2D) materials within the GW self-energy approximation has proven to be a rather demanding computational task. The main reason is the strong $q$ dependence of the 2D dielectric function around $q = 0$ that calls for a much denser sampling of the Brillouin zone (BZ) than is necessary for similar three-dimensional solids. Here, we use an analytical expression for the small $q$ limit of the 2D response function to perform the BZ integral over the critical region around $q = 0$. This drastically reduces the requirements on the $q$-point mesh and implies a significant computational speedup. For example, in the case of monolayer MoS$_2$, convergence of the $G_0W_0$ band gap to within similar to 0.1 eV is achieved with 12 x 12 $q$ points rather than the 36 x 36 mesh required with discrete BZ sampling techniques. We perform a critical assessment of the band gap of the three prototypical 2D semiconductors, MoS$_2$, h-BN, and phosphorene, including the effect of self-consistency at the GW$_0$ level. The method is implemented in the open source code GPAW.

**General information**

**State:** Published

**Organisations:** Center for Nanostructured Graphene, Department of Physics, Theoretical Atomic-scale Physics

**Authors:** Rasmussen, F. A. (Intern), Schmidt, P. S. (Intern), Winther, K. T. (Intern), Thygesen, K. S. (Intern)

**Number of pages:** 9

**Publication date:** 2016

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

**Publication information**

**Journal:** Physical Review B

**Volume:** 94

**Issue number:** 15

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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
Elastic interaction between twins during tensile deformation of austenitic stainless steel

In austenite, the twin boundary normal is a common elastically stiff direction shared by the two twins, which may induce special interactions. By means of three-dimensional X-ray diffraction this elastic interaction has been analysed and compared to grains separated by conventional grain boundaries. However, the components of the Type II stress normal to the twin boundary plane exhibit the same large variations as for the grain boundaries. Elastic grain interactions are therefore complex and must involve the entire set of neighbouring grains. The elastic-regime stress along the tensile direction qualitatively depends on the grain orientation, but grain-to-grain variations are large.
Electrochemical Oxidation of Hydrocarbons for Green Chemistry

General information
State: Published
Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics
Authors: Winiwarter, A. (Intern), Stephens, I. (Intern), Chorkendorff, I. (Intern)
Number of pages: 1
Publication date: 2016
Main Research Area: Technical/natural sciences
Links:
http://www.sustain.dtu.dk/

Bibliographical note
Sustain Abstract P-9
Publication: Research - peer-review › Conference abstract for conference – 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

Electron Transfer and Solvent-Mediated Electronic Localization in Molecular Photocatalysis
This work provides a detailed mechanism for electron transfer in a heterodinuclear complex designed as a model system in which to study homogeneous molecular photocatalysis. With efficient Born–Oppenheimer molecular dynamics simulations, we show how intermediate, charge-separated states can mediate the electron transfer. We observe how Jahn–Teller distortion effects play out in solution, when the molecule has energetically close-lying states, and how this distortion is averaged out in the thermal sampling. Finally, we demonstrate how the solvent helps stabilize and localize the separated charge. The information on the electronic configuration and separate states is of key importance for designing next-generation photocatalysts.

General information
State: Published
Elucidating oxygen electrocatalysis with synchrotron X-rays: PEM fuel cells and electrolyzers: An experimental study

In this thesis electrocatalysts for the oxygen reduction reaction (ORR) and the oxygen evolution reaction (OER) have been investigated using synchrotron based X-ray diffraction and X-ray absorption spectroscopy methods. The catalysts are based on Pt alloys and RuO2 for ORR and OER, respectively.

For ORR model systems of PtxGd and PtxY alloys were fabricated. EXAFS were measured on a range of size-selected PtxGd nanoparticles to determine the interatomic Pt-Pt distances. The larger particles with a diameter of 8 nm were most active with a mass activity of 3.5 A/mgPt, and these particles also showed the greatest compression of the Pt-Pt nearest neighbor distance. This is consistent with the formation of a pure Pt overlayer that is compressed relative to bulk Pt, which explains the increase in activity purely due to strain effects. The activity of the different sized nanoparticles was correlated to the compression; the smaller particles are less active and has a lower degree of compression.

To get more insight into the Pt overlayer single crystal model systems of Gd/Pt(111) and Y/Pt(111) were fabricated by depositing films of Gd or Y on a Pt(111) single crystal at high temperatures in UHV. XRD measurements on both model systems showed the formation of an FCC-like overlayer about 3 atomic layers thick on Y/Pt(111) and about 5 layers thick on Gd/Pt(111). The average in-plane compression on the two systems were 1.4% and 0.31% respectively. The XRD analysis also revealed a possible high degree of micro-strain, which can explain why both model systems have similar ORR activity despite their large difference in average compression.

An in-situ XRD study of Gd/Pt(111) showed that the overlayer forms immediately upon exposure to acidic electrolyte at open circuit potential. Furthermore stability measurements showed that the in-plane compression relaxes during the first 2000-3000 cycles, explaining the loss of activity primarily in this range of cycling.

For OER mass-selected nanoparticles of metallic Ru and thermally oxidized RuO2 were fabricated. Both materials are highly active for OER, although the metallic Ru nanoparticles exceptionally so. However this comes as a trade-off in stability, as the metallic particles dissolves rapidly at OER conditions. In an in-situ XAS experiment the oxidation state of the nanoparticles were tracked as a function of potential. It was found that the metallic nanoparticles strongly oxidize around 1.1 V vs. RHE. Furthermore, from the measurements of both types of nanoparticles we hypothesize that RuO2 binds O too strongly, as an increase in potential leads to further oxidation of Ru. As a consequence of too strong binding of O, the oxidation state of Ru decrease during OER as the coverage of O intermediates are no longer based on thermodynamics but rather kinetics.

Finally an IrO2 protection layer on a RuO2 thin film catalyst was investigated using high resolution XAS. It was found that the stability of the RuO2 thin film catalyst was improved by adding small amounts of IrO2 on the surface. With in-situ XAS measurements we were able to measure the oxidation state of Ir as a function of applied potential. It was found that the IrO2 does not participate in the OER, but sits at the surface and takes up oxygen by increasing its oxidation state.
Recent upgrades to the FIDA (fast-ion D-alpha) diagnostic at ASDEX Upgrade are discussed. The diagnostic has been extended from three to five line of sight arrays with different angles to the magnetic field, and a spectrometer redesign allows the simultaneous measurement of red- and blue-shifted parts of the Doppler spectrum. These improvements make it possible to reconstruct the 2D fast-ion velocity distribution from the FIDA measurements by tomographic inversion under a wide range of plasma parameters. Two applications of the tomography are presented: a comparison between the distributions resulting from 60 keV and 93 keV neutral beam injection and a velocity-space resolved study of fast-ion redistribution induced by a sawtooth crash inside and outside the sawtooth inversion radius.
ETEM characterization of NiGa model catalysts for CO$_2$ hydrogenation to Methanol

General information
State: Published
Organisations: Center for Electron Nanoscopy, Department of Physics, Experimental Surface and Nanomaterials Physics
Publication date: 2016
Main Research Area: Technical/natural sciences
Electronic versions:
EMCAT_1.pdf

Bibliographical note
For poster presentation
Source: PublicationPreSubmission
Source-ID: 277080137
Publication: Research - peer-review › Journal article – Annual report year: 2016

Evidence of a Jahn-Teller impurity in a cubic lattice displaying a compressed geometry

General information
State: Published
Organisations: Department of Physics, Theoretical Atomic-scale Physics, Universidad de Cantabria
Authors: García-Fernandez, P. (Ekstern), Aramburu, J. (Ekstern), García Lastra, J. M. (Intern), Moreno, M. (Ekstern)
Exciton ionization in multilayer transition-metal dichalcogenides

Photodetectors and solar cells based on materials with strongly bound excitons rely crucially on field-assisted exciton ionization. We study the ionization process in multilayer transition-metal dichalcogenides (TMDs) within the Mott-Wannier model incorporating fully the pronounced anisotropy of these materials. Using complex scaling, we show that the field-dependence of the ionization process is strongly dependent on orientation. Also, we find that direct and indirect excitons behave qualitatively differently as a result of opposite effective anisotropy of these states. Based on first-principles material parameters, an analysis of several important TMDs reveals WSe$_2$ and MoSe$_2$ to be superior for applications relying on ionization of direct and indirect excitons, respectively.
Excitons in van der Waals Heterostructures: A theoretical study

Van der Waals heterostructures (vdWHs) represent a novel and largely unexplored class of materials. Since 2013, when Geim and Grigorieva first conceived the stacking of 2D (two-dimensional) materials to create artificial layered structures with tailored properties, a number of promising (opto)electronics devices, e.g. light emitting diodes, solar cells, ultra-fast photodetectors, transistors etc., have been successfully fabricated. It is well established that for isolated 2D semiconductors and vdWHs the optical response is governed by excitonic effects. While it is understood that the reduced amount of electronic screening in freestanding 2D materials is the main origin of extraordinarily strongly bound excitons, a theoretical understanding of excitonic effects and of how the electronic screening is affected for the more complex case of multi-layer structures is still lacking due to the computational limitations of standard ab-initio methods.

In this thesis first-principles models that overcome the limitations of standard ab-initio techniques are developed for the description of dielectric, electronic and excitonic properties in isolated 2D materials and vdWHs. The main contribution is a multi-scale method that seemingly connects the excitonic effects in the monolayer limit to the more challenging case of multi-layered structures. The method is based on the analogy between vdWHs and the popular construction toy Lego. This analogy is much deeper than one would first expect: it is possible to predict the dielectric properties of a vdWH from the dielectric functions of the individual 2D layers, which represent the dielectric genome of the heterostructure. From the vdWH dielectric properties one evaluates the screened interaction between the electron and hole forming the exciton which can then be used in a generalized hydrogenic model to compute exciton binding energies in isolated, supported, or encapsulated 2D semiconductors. The non-locality of the dielectric screening is inherently included in our method and we can successfully describe the non-hydrogenic Rydberg series of low-dimensional systems. This multi-scale method also proves successful when combined with many-body perturbation techniques for accurate prediction of electronic band structure or with complex scaling techniques for exciton dissociation rates in vdWHs. The validity of our techniques is demonstrated through numerous comparison to experimental results.

Ultimately this thesis puts forth a first-principles methodology that allows us to address scientific questions that are beyond the capability of existing state of the art techniques and enables 2D materials researcher to predict and design dielectric, electronic and excitonic properties of general vdWHs.
Experimental characterization of a prototype secondary spectrometer for vertically scattering multiple energy analysis at cold-neutron triple axis spectrometers

A thorough experimental characterization of a multiplexing backend with multiple energy analysis on a cold-neutron triple axis spectrometer (cTAS) is presented. The prototype employs two angular segments (2 theta-segments) each containing five vertically scattering analyzers (energy channels), which simultaneously probe an energy transfer range of 2 meV at the corresponding two scattering angles. The feasibility and strength of such a vertically scattering multiple energy analysis setup is clearly demonstrated. It is shown, that the energy resolution near the elastic line is comparable to the energy resolution of a standard cTAS. The dispersion relation of the antiferromagnetic excitations in MnF2 has been mapped out by performing constant energy transfer maps. These results show that the tested setup is virtually spurion free. In addition, focusing effects due to (mis)matching of the instrumental resolution ellipsoid to the excitation branch are clearly evident. (C) 2016 Elsevier B.V. All rights reserved.
**Experimental characterization of Raman overlaps between mode-groups**

Mode-division multiplexing has the potential to further increase data transmission capacity through optical fibers. In addition, distributed Raman amplification is a promising candidate for multi-mode signal amplification due to its desirable noise properties and the possibility of mode-equalized gain. In this paper, we present an experimental characterization of the intermodal Raman intensity overlaps of a few-mode fiber using backward-pumped Raman amplification. By varying the input pump power and the degree of higher order mode-excitation for the pump and the signal in a 10km long two-mode fiber, we are able to characterize all intermodal Raman intensity overlaps. Using these results, we perform a Raman amplification measurement and demonstrate a mode-differential gain of only 0.25dB per 10dB overall gain. This is, to the best of our knowledge, the lowest mode differential gain achieved for amplification of mode division multiplexed signals in a single fiber.
Experimental Elucidation of the Oxygen Reduction Volcano In Base on a Pt Alloy Single Crystal

It is of fundamental importance to understand the factors controlling trends in activity for electrocatalytic reactions as a function of pH. In the case of the oxygen reduction reaction, numerous reports suggest significant divergences between noble metals surface catalytic performances in acid and base.[1,2]

In our earlier studies, we mapped out the experimental Sabatier volcano for the oxygen reduction reaction in 0.1 M HClO4
using the Cu/Pt(111) near-surface alloy system, see Figure 1 for near-surface alloy schematic.[3,4]

In this study, as those of [3,4], we found that by changing the subsurface coverage of Cu we could tune the surface binding of the key reaction intermediate, OH; we thus monitored the OH binding energy shift through the observable shifts in the base voltammograms in both acidic and alkaline media.

Further, we elucidate the experimental oxygen reduction volcano in 0.1 M KOH for the Cu/Pt(111) near-surface alloy system. Remarkably, we observe that the same trend persists between OH binding shifts and Cu/Pt(111) oxygen reduction activities between acid and alkaline electrolyte, with the optimum catalyst in alkaline exhibiting an 8-fold improvement in activity, relative to Pt(111). However, all surfaces show a ~4 fold improvement in activity in 0.1 M KOH, relative to the same surface in 0.1 M HClO4. At the peak of the volcano the surface exhibits an exceptionally high specific activity of 90 mA/cm2 at 0.9 V with respect to the reversible hydrogen electrode. Thus, our results confirm that OH binding energy is the key descriptor in both alkaline and acid electrolytes.

General information
State: Published
Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics, Ruhr-Universität Bochum, Technische Universität München
Authors: Jensen, K. D. (Intern), Tymoczko, J. (Ekstern), Bandarenka, A. S. (Ekstern), Chorkendorff, I. (Intern), Escribano, M. E. (Intern), Stephens, I. (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

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Article number: 2436
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http://ma.ecsdl.org.proxy.findit.dtu.dk/content/MA2016-02/38/2436.abstract?sid=06bf69ab-f635-4937-b27d-21bfe0f4c5c7
Publication: Research - peer-review › Conference abstract in journal – Annual report year: 2016

Exploiting the energy source of the stars: Fusion energy research at DTU
With increasing energy demands and a limited supply of fossil fuels, the need for efficient, clean, and sustainable energy sources grows ever more pressing. Nuclear fusion – the process from which stars like the Sun derive their energy – holds the potential to help address this challenge. To mimic this process on earth, experimental fusion devices seek to confine and heat gas to millions of degrees (creating a fusion plasma). Learning how such plasmas behave is a crucial step towards realizing fusion as a sustainable energy source. At the Plasma Physics and Fusion Energy (PPFE) section at DTU Physics, we are exploring this issue, focusing on three areas of high priority on the way towards a working fusion power plant.

General information
State: Published
Organisations: Department of Physics, Plasma Physics and Fusion Energy
Number of pages: 1
Publication date: 2016
Main Research Area: Technical/natural sciences
Links:
http://www.sustain.dtu.dk/

Bibliographical note
Sustain Abstract E-10
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2016

Exploring the Lanthanide Contraction to Tune the Activity and Stability of Pt
The high platinum loadings required to compensate for the slow kinetics of the oxygen reduction reaction (ORR) impede the widespread uptake of polymer electrolyte membrane fuel cells. In order to improve the ORR kinetics and reduce the Pt...
loading, we can tailor the electronic properties of the Pt surface atoms by means of alloying Pt with other metals. Researchers have intensively studied alloys of Pt with late transition metals such as Ni and Co during the last decades. However, these compounds typically degrade under fuel cell reaction conditions, due to dealloying. In contrast, alloys of Pt and lanthanides present very negative enthalpy of formation [1,2], which should increase their resistance to degradation.

General information
State: Published
Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics, Theoretical Atomic-scale Physics, University of Copenhagen
Publication date: 2016
Conference: PRIME 2016/230th ECS Meeting, Honolulu, United States, 02/10/2016 - 02/10/2016
Main Research Area: Technical/natural sciences

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Journal: Electrochemical Society. Meeting Abstracts (Online)
Volume: MA2016-02
Article number: 2403
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Publication: Research - peer-review » Conference abstract in journal – Annual report year: 2016

Eye-safe diode laser Doppler lidar with a MEMS beam-scanner
We present a novel Doppler lidar that employs a cw diode laser operating at 1.5 μm and a micro-electro-mechanical-system scanning mirror (MEMS-SM). In this work, two functionalities of the lidar system are demonstrated. Firstly, we describe the capability to effectively steer the lidar probe beam to multiple optical transceivers along separate lines-of-sight. The beam steering functionality is demonstrated using four lines-of-sight – each at an angle of 18° with respect to their symmetry axis. Secondly, we demonstrate the ability to spatially dither the beam focus to reduce the mean irradiance at the probing distance (R = 60 m) of each line-of-sight – relevant for meeting eye-safety requirements. The switching time of the MEMS-SM is measured to be in the order of a few milliseconds. Time-shared (0.25 s per line-of-sight) radial wind speed measurements at 50 Hz data rate are experimentally demonstrated. Spatial dithering of the beam focus is also implemented using a spiral scan trajectory resulting in a 16 dB reduction of beam focus mean irradiance.

General information
State: Published
Organisations: Department of Photonics Engineering, Optical Sensor Technology, Department of Physics, Risø National Laboratory for Sustainable Energy
Authors: Hu, Q. (Intern), Pedersen, C. (Intern), Rodrigo, P. J. (Intern)
Number of pages: 1
Pages: 1934
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Optics Express
Volume: 24
Issue number: 3
ISSN (Print): 1094-4087
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): SJR 1.519 SNIP 1.567 CiteScore 3.74
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.48 SJR 1.532 SNIP 1.544
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.91 SNIP 1.674 CiteScore 3.78
Factors Contributing to Activity in Catalytic Soot Oxidation

General information
State: Published
Fast-ion energy resolution by one-step reaction gamma-ray spectrometry

The spectral broadening of γ-rays from fusion plasmas can be measured in high-resolution gamma-ray spectrometry (GRS). We derive weight functions that determine the observable velocity space and quantify the velocity-space sensitivity of one-step reaction high-resolution GRS measurements in magnetized fusion plasmas. The weight functions suggest that GRS resolves the energies of fast ions directly, without the need for tomographic inversion for selected one-step reactions at moderate plasma temperatures. The D(p,γ)3He reaction allows the best direct fast-ion energy resolution. We illustrate our general formalism using reactions with and without intrinsic broadening of the γ-rays for the GRS diagnostic at JET.
Femtosecond X-ray absorption and emission spectroscopy on ZnO nanoparticles in solution

We have performed femtosecond X-ray spectroscopy measurements after UV photoexcitation of a colloidal solution of ZnO nanoparticles. The results indicate sub-ps hole trapping at oxygen vacancies with shallowly-trapped electrons in the conduction band.

General information

State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics
Number of pages: 3
Publication date: 2016

Host publication information
Title of host publication: International Conference on Ultrafast Phenomena
Femtosecond X-Ray Scattering Study of Ultrafast Photoinduced Structural Dynamics in Solvated [Co(terpy)$_2$]$_2^{2+}$

We study the structural dynamics of photoexcited [Co(terpy)$_2$]$_2^{2+}$ in an aqueous solution with ultrafast x-ray diffuse scattering experiments conducted at the Linac Coherent Light Source. Through direct comparisons with density functional theory calculations, our analysis shows that the photoexcitation event leads to elongation of the Co-N bonds, followed by coherent Co-N bond length oscillations arising from the impulsive excitation of a vibrational mode dominated by the symmetrical stretch of all six Co-N bonds. This mode has a period of 0.33 ps and decays on a subpicosecond time scale. We find that the equilibrium bond-elongated structure of the high spin state is established on a single-picosecond time scale and that this state has a lifetime of ∼7 ps.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Theoretical Atomic-scale Physics, Department of Chemistry, Lund University
Number of pages: 6
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Physical Review Letters
Volume: 117
Issue number: 1
Article number: 013002
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
FeNi/Y-Al₂O₃ Egg-shell Catalyst for H₂ Generation by Ammonia Decomposition

General information
State: Published
Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics, Center for Electron Nanoscopy, Neutrons and X-rays for Materials Physics
Publication date: 2016
Main Research Area: Technical/natural sciences
Electronic versions:
C.Damsgaard_NSC2016_poster.pdf

Bibliographical note
P-80
Fine-tuning the activity of oxygen evolution catalysts: The effect of oxidation pre-treatment on size-selected Ru nanoparticles

Water splitting is hindered by the sluggish kinetics of the oxygen evolution reaction (OER). The choice of materials for this reaction in acid is limited to the platinum group metals; high loading required of these scarce and expensive elements severely limit the scalability of such technology. Ruthenium oxide is among the best catalysts for OER, however the reported activity and stability can vary tremendously depending on the preparation conditions and pre-treatment. Herein, we investigate the effect of oxidation treatment on mass-selected Ru nanoparticles in the size range between 2 and 10 nm. The effect of two distinct oxidation pre-treatments on the activity and stability have been investigated: (1) thermal oxidation; and (2) oxidation with an oxygen plasma under vacuum. We report that activity and stability can be tuned by using different oxidation pre-treatments. Thermally oxidized particles exhibited the lowest activity, although over an order of magnitude higher than the state of the art, and the highest stability. Plasma-treated particles showed intermediate performance between as-deposited and thermally oxidized NPs.

General information
State: Published
Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics, Center for Electron Nanoscopy
Number of pages: 8
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Journal: Catalysis Today
Volume: 262
ISSN (Print): 0920-5861
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BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 1.329 SJR 1.347 CiteScore 4.55
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.26 SJR 1.322 SNIP 1.369
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.335 SNIP 1.403 CiteScore 4
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.315 SNIP 1.453 CiteScore 3.72
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.299 SNIP 1.415 CiteScore 3.9
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.469 SNIP 1.422 CiteScore 3.38
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.472 SNIP 1.562 CiteScore 3.34
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.761 SNIP 1.449
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): SJR 2.135 SNIP 1.147 CiteScore 4.58
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.48 SJR 1.964 SNIP 1.195
First Principles Calculations of Electronic Excitations in 2D Materials

Since the first reported synthesis of graphene - an atomically thin carbon material - in 2004 there has been a surge of research in discovering other novel two-dimensional materials. The reason is clear: two-dimensional materials are thought to be able to lead to new fast and low-power ultra-thin electronics and high efficiency solar cells. Contrary to many other nano-materials, methods for large scale fabrication and patterning have already been demonstrated and the first real technological applications have already be showcased. Still the technology is very young and the number of well-studied 2D materials are few. However as the list of 2D materials is growing it is necessary to investigate their fundamental structural, electronic and optical properties. These are determined by the atomic and electronic structure of the materials that can quite accurately predicted by computational quantum mechanics methods.

One of these methods, Density Functional Theory (DFT), has been very successful at determining structural properties of 2D materials. It is however well-known that it less accurate when it comes to predicting the energy levels of excited states that are important in order to determine electronic transport, optical and chemical properties. On the other hand it has shown to be a great starting point for a systematic perturbation theory approach to obtain the so-called quasiparticle spectrum. In the GW approximation one considers the potential from a charged quasiparticle as if it is being
screened by the electrons in the material. This method has been very successful for calculating quasiparticle energies of bulk materials but results have been more varying for 2D materials. The reason is that the 2D confined electrons are less able to screen the added charge and some of the numerical methods that are efficient for bulk systems become invalid. In this thesis I describe the study of a set of novel 2D materials and establish their electronic and optical properties using DFT and the GW approximation while taking the reduced screening properly into account as well as taking regard to other numerical problems that have often been neglected. Secondly I show how one can efficiently take the 2D nature into account in the GW approximation and thereby make future calculations require much less computational resources.

General information
State: Published
Organisations: Department of Physics
Authors: Rasmussen, F. A. (Intern), Thygesen, K. S. (Intern)
Number of pages: 162
Publication date: 2016

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Publisher: Department of Physics, Technical University of Denmark
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
Thesis.pdf

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Projects:
First Principles Calculations of Electronic Excitations in 2D Materials
Publication: Research › Ph.D. thesis – Annual report year: 2016

Fluxon Dynamics in Elliptic Annular Josephson Junctions
We analyze the dynamics of a magnetic flux quantum (current vortex) trapped in a current-biased long planar elliptic annular Josephson tunnel junction. The system is modeled by a perturbed sine-Gordon equation that determines the spatial and temporal behavior of the phase difference across the tunnel barrier separating the two superconducting electrodes. In the absence of an external magnetic field, the fluxon dynamics in an elliptic annulus does not differ from that of a circular annulus where the stationary fluxon speed merely is determined by the system losses. The interaction between the vortex magnetic moment and a spatially homogeneous in-plane magnetic field gives rise to a tunable periodic non-sinusoidal potential which is strongly dependent on the annulus aspect ratio. We study the escape of the vortex from a well in the tilted potential when the bias current exceeds the depinning current. The smallest depinning current as well as the lowest sensitivity of the annulus to the external field is achieved when the axes ratio is equal to root 2. The presented extensive numerical results are in good agreement with the findings of the perturbative approach. We also probe the rectifying properties of an asymmetric potential implemented with an egg-shaped annulus formed by two semi-elliptic arcs.

General information
State: Published
Organisations: Department of Physics, Consiglio Nazionale delle Ricerche
Authors: Monaco, R. (Ekstern), Mygind, J. (Intern)
Number of pages: 13
Pages: 1-13
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Low Temperature Physics
Volume: 183
Issue number: 1-2
ISSN (Print): 0022-2291
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 0.583 SJR 0.471 CiteScore 0.96
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 0.95 SJR 0.461 SNIP 0.797
Web of Science (2016): Indexed yes
Frequency tuning of single photons from a whispering-gallery mode resonator to MHz-wide transitions

Quantum repeaters rely on interfacing flying qubits with quantum memories. The most common implementations include a narrowband single photon matched in bandwidth and central frequency to an atomic system. Previously, we demonstrated the compatibility of our versatile source of heralded single photons, which is based on parametric down-conversion in a triply resonant whispering-gallery mode resonator, with alkaline transitions [Schunk et al., Optica 2015, 2, 773]. In this paper, we analyse our source in terms of phase matching, available wavelength-tuning mechanisms and applications to narrowband atomic systems. We resonantly address the D1 transitions of caesium and rubidium with this optical parametric oscillator pumped above its oscillation threshold. Below threshold, the efficient coupling of single photons to atomic transitions heralded by single telecom-band photons is demonstrated. Finally, we present an accurate analytical description of our observations. Providing the demonstrated flexibility in connecting various atomic transitions with telecom wavelengths, we show a promising approach to realize an essential building block for quantum repeaters.

General information
State: Published
Organisations: Quantum Physics and Information Technology, Friedrich-Alexander University Erlangen-Nuremberg, University of Otago
Full-field hard x-ray microscopy with interdigitated silicon lenses

Full-field x-ray microscopy using x-ray objectives has become a mainstay of the biological and materials sciences. However, the inefficiency of existing objectives at x-ray energies above 15 keV has limited the technique to weakly absorbing or two-dimensional (2D) samples. Here, we show that significant gains in numerical aperture and spatial resolution may be possible at hard x-ray energies by using silicon-based optics comprising ‘interdigitated’ refractive silicon lenslets that alternate their focus between the horizontal and vertical directions. By capitalizing on the nano-manufacturing processes available to silicon, we show that it is possible to overcome the inherent inefficiencies of silicon-based optics and interdigitated geometries. As a proof-of-concept of Si-based interdigitated objectives, we demonstrate a prototype interdigitated lens with a resolution of ≈255 nm at 17 keV.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, DTU Danchip, Experimental Surface and Nanomaterials Physics, Department of Micro- and Nanotechnology, Silicon Microtechnology, European Synchrotron Radiation Facility
Pages: 460-464
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
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ISSN (Print): 0030-4018
Ratings:
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): SNIP 0.95 SJR 0.614 CiteScore 1.86
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 1.65 SJR 0.603 SNIP 0.87
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.673 SNIP 0.928 CiteScore 1.62
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 0.7 SNIP 1.03 CiteScore 1.62
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 0.74 SNIP 1.154 CiteScore 1.78
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 0.801 SNIP 1.125 CiteScore 1.63
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 0.811 SNIP 1.2 CiteScore 1.62
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Heterogeneous catalysis, the conversion of chemicals by the use of a suitable solid state catalyst, is a very important technology in modern society and it is involved in the production of up to 90% of all chemicals. Catalysis has in this way played a significant role in the technological and economic development in the 20th century. There is however a downside to this development and we are seeing significant pollution and pressure on resources. Catalysis therefore has an increasingly important role in limiting pollution and optimizing the use of resources. This development will depend on our fundamental understanding of catalytic processes and our ability to make use of that understanding.

This thesis presents fundamental studies of catalyst nanoparticles with particular focus on dynamic processes. Such studies often require atomic-scale characterization, because the catalytic conversion takes place on the molecular and atomic level.

Transmission electron microscopy (TEM) has the ability to image nanostructures with atomic resolution and reveal the atomic configuration of the important nanoparticle surfaces. In the present work, TEM has been used to study nanoparticles in situ at elevated temperature and with gas present in the microscope in order to recreate the conditions found in a chemical reactor. This is very important because we know that particles may change shape as their surfaces respond to a changing gas atmosphere. To obtain quantitative and credible information in situ, it is very important that we only study intrinsic structures and phenomena and not those that may be induced by the high energy electrons used to image the specimen. This requires careful consideration of the influence of the electron beam in order to understand, control and minimize that influence.

I present four different topics, each related to different aspects of nanoparticle dynamics and catalysis. The first topic is the reduction of a homogeneous solid state precursor to form the catalytically active phase which is metal nanoparticles on an inert support. Here, we have reduced Cu phyllosilicate to Cu on silica and imaged the process in situ. The data obtained established the foundation for modeling work which revealed that the reduction proceeded by an autocatalytic route. Here, the initial nucleation of Cu is slow and the subsequent growth in size is fast because the Cu particles themselves catalyze further reduction.

The second topic treated the active state of a methanol synthesis catalyst. This work was performed by a parallel
approach, where we investigated identically created nanoparticles both with TEM and X-ray photoelectron spectroscopy (XPS). The methanol synthesis catalyst is a complex high surface area Cu=ZnO=Al2O3 structure that is difficult to study by TEM. We therefore created size-selected CuZn alloy nanoparticles that were transformed by oxidation and reduction into Cu nanoparticles decorated with ZnO. This represents a simplified model system for the high surface area catalyst. The interplay between Cu and ZnO and the exact role of ZnO as a promoter for catalytic activity is not yet fully understood. Our work revealed that the surface of the reduced catalyst consists mainly of Cu decorated with well defined ZnO crystals. It was demonstrated by XPS that a fraction of the ZnO is reduced simultaneously with the Cu under H2 atmosphere, presumably forming a surface alloy in the Cu.

The third topic studied the sintering of Cu nanoparticles supported on silica. Sintering is the main deactivation mechanism for the methanol synthesis catalyst and so this topic is of great interest to the development of better catalysts. It was found that sintering proceeded via Ostwald ripening, i. e. the migration of atomic species between particles, with a net flow from small to larger particles resulting in an overall growth in particle size. The presence of CO increased the rate of sintering significantly and the presence of H2O slowed it down.

The fourth topic investigated the oxidation of CO on a Pt catalyst in the special case where the reaction displays temporal rate oscillations under fixed conditions. This is a well-known phenomenon, but the mechanism driving the oscillations on nanoparticles has hitherto been unknown. We used nanoreactor technology which allows for simultaneous TEM imaging and activity measurement, also referred to as an Operando experiment. With this we revealed that the shape of the Pt nanoparticles changed in phase with changes in global reaction rate. By the use of reactor modeling it was possible to show that the oscillations were possible due to the coupling between the self-poisoning nature of the CO oxidation reaction on Pt and gas flow and diffusion in the reactor. Our work showed that shape changes can drive global rate oscillations.

**General information**

State: Published
Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics, Haldor Topsoe AS
Authors: Elkjær, C. F. (Intern), Chorkendorff, I. (Intern), Helveg, S. (Ekstern), Sehested, J. (Ekstern)
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Publication date: 2016

**Publication information**

Publisher: Department of Physics, Technical University of Denmark
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
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**Relations**

Projects:
Fundamental investigations of catalyst nanoparticles
Publication: Research › Ph.D. thesis – Annual report year: 2016

**Gas puff fuelling simulation with a combined neutral/HESEL model**

**General information**

State: Published
Organisations: Department of Physics, Plasma Physics and Fusion Energy
Authors: Thrysøe, A. S. (Intern), Madsen, J. (Intern), Naulin, V. (Intern), Nielsen, A. H. (Intern), Rasmussen, J. J. (Intern)
Number of pages: 1
Publication date: 2016
Main Research Area: Technical/natural sciences
Electronic versions:
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Source: PublicationPreSubmission
Source-ID: 128545650
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**Global Energy Consumption: The Numbers for Now and in the Future**

**General information**

State: Published
Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics
Authors: Seger, B. (Intern)
Publication date: 2016
GRB 980425 host: [C II], [O I], and CO lines reveal recent enhancement of star formation due to atomic gas inflow

Context. Accretion of gas from the intergalactic medium is required to fuel star formation in galaxies. We have recently suggested that this process can be studied using host galaxies of gamma-ray bursts (GRBs).

Aims. Our aim is to test this possibility by studying in detail the properties of gas in the closest galaxy hosting a GRB (980425).

Methods. We obtained the first ever far-infrared (FIR) line observations of a GRB host, namely Herschel/PACS resolved [C ii] 158 μm and [O i] 63 μm spectroscopy, and an APEX/SHeFI CO(2-1) line detection and ALMA CO(1-0) observations of the GRB 980425 host.

Results. The GRB 980425 host has elevated [C ii]/FIR and [O i]/FIR ratios and higher values of star formation rates (SFR) derived from line ([C ii], [O i], Hα) than from continuum (UV, IR, radio) indicators. [C ii] emission exhibits a normal morphology, peaking at the galaxy centre, whereas [O i] is concentrated close to the GRB position and the nearby Wolf-Rayet region. The high [O i] flux indicates that there is high radiation field and high gas density at these positions, as derived from modelling of photo-dissociation regions. The [C ii]/CO luminosity ratio of the GRB 980425 host is close to the highest values found for local star-forming galaxies. Indeed, its CO-derived molecular gas mass is low given its SFR and metallicity, but the [C ii]-derived molecular gas mass is close to the expected value.

Conclusions. The [O i] and H i concentrations and the high radiation field and density close to the GRB position are consistent with the hypothesis of a very recent (at most a few tens of Myr ago) inflow of atomic gas triggering star formation. In this scenario dust has not had time to build up (explaining high line-to-continuum ratios). Such a recent enhancement of star formation activity would indeed manifest itself in high SFR_{line}/SFR_{continuum} ratios because the line indicators are sensitive only to recent (∼ 10 Myr) activity, whereas the continuum indicators measure the SFR averaged over much longer periods (∼100 Myr). Within a sample of 32 other GRB hosts, 20 exhibit SFR_{line}/SFR_{continuum} > 1 with a mean ratio of 1.74 ± 0.32. This is consistent with a very recent enhancement of star formation that is common among GRB hosts, so galaxies that have recently experienced inflow of gas may preferentially host stars exploding as GRBs. Therefore GRBs may be used to select a unique sample of galaxies that is suitable for the investigation of recent gas accretion.

General information
State: Published
Organisations: Department of Physics, Plasma Physics and Fusion Energy, University of Edinburgh, European Space Agency, University of Copenhagen, Nicolaus Copernicus University in Torun, Universidade de Lisboa, Leiden University, Osservatorio Astrofisico Di Arcetri, Florence, Universiteit Gent, Instituto de Astrofísica de Andalucía, Vrije Universiteit Amsterdam, European Space Astronomy Centre and European Space Agency, Thüringer Landessternwarte Tautenburg, Centro de Astrobiología, National Institute for Astrophysics, Max-Planck-Institut fur extraterrestrische Physik, Stockholm University, Chinese Academy of Sciences
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Main Research Area: Technical/natural sciences

Publications information
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): SJR 2.265 SNIP 1.099 CiteScore 3.8
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.68 SJR 2.234 SNIP 1.199
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 2.545 SNIP 1.224 CiteScore 3.5
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.883 SNIP 1.247 CiteScore 2.82
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.747 SNIP 1.159 CiteScore 2.01
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 2.903 SNIP 1.36 CiteScore 3.14
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 2.737 SNIP 1.322 CiteScore 3.42
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 2.849 SNIP 1.424
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.976 SNIP 1.438
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 2.907 SNIP 1.291
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 2.861 SNIP 1.333
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 3.646 SNIP 1.4
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 3.265 SNIP 1.338
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 2.862 SNIP 1.448
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 2.157 SNIP 1.362
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 1.845 SNIP 1.35
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 1.607 SNIP 0.736
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 2.439 SNIP 1.04
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 2.478 SNIP 1.07

Original language: English
Dust, extinction, Galaxies: individual: ESO 184-G82, Galaxies: ISM, Galaxies: star formation, Gamma-ray burst: individual: 980425, Submillimeter: galaxies
Electronic versions: 1609.01742v1.pdf. Embargo ended: 04/05/2017
Green high-power tunable external-cavity GaN diode laser at 515 nm
A 480 mW green tunable diode laser system is demonstrated for the first time to our knowledge. The laser system is based on a GaN broad-area diode laser and Littrow external-cavity feedback. The green laser system is operated in two modes by switching the polarization direction of the laser beam incident on the grating. When the laser beam is p-polarized, an output power of 50 mW with a tunable range of 9.2 nm is achieved. When the laser beam is s-polarized, an output power of 480 mW with a tunable range of 2.1 nm is obtained. This constitutes the highest output power from a tunable green diode laser system.

General information
State: Published
Organisations: Department of Photonics Engineering, Diode Lasers and LED Systems, Department of Applied Mathematics and Computer Science, Department of Physics
Authors: Chi, M. (Intern), Jensen, O. B. (Intern), Petersen, P. M. (Intern)
Pages: 4154-4157
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Optics Letters
Volume: 41
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ISSN (Print): 0146-9592
Ratings: BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 3.89 SJR 1.79 SNIP 1.597
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.54 SJR 1.769 SNIP 1.549
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 2.013 SNIP 1.53 CiteScore 3.53
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.429 SNIP 1.997 CiteScore 3.86
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.441 SNIP 2.058 CiteScore 3.95
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 2.577 SNIP 1.92 CiteScore 3.52
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 2.519 SNIP 2.453 CiteScore 3.69
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 2.637 SNIP 2.263
Web of Science (2010): Indexed yes
Halogen-Bonding-Assisted Iodosylbenzene Activation by a Homogenous Iron Catalyst

The iron(III) complex of hexadentate N,N,N′-tris(2-pyridylmethyl)ethylendiamine-N′-acetate (tpena⁻) is a more effective homogenous catalyst for selective sulfoxidation and epoxidation with insoluble iodosylbenzene, [PhIO]ₙ, compared with soluble methyl-morpholine-N-oxide (NMO). We propose that two molecules of [Fe(tpena)]²⁺ cooperate to solubilize PhIO, extracting two equivalents to form the halogen-bonded dimeric ([Fe(tpena)OIPh]₂)⁴⁺. The closest intradimeric I⋯O distance, 2.56 Å, is nearly 1 Å less than the sum of the van de Waals radii of these atoms. A correlation of the rates of the reaction of ([Fe(tpena)OIPh]₂)⁴⁺ with para-substituted thioanisoles indicate that this species is a direct metal-based oxidant rather than a derived ferryl or perferryl complex. A study of gas-phase reactions indicate that an ion at m/z=231.06100 originates from solution-state ([Fe(tpena)OIPh]₂)⁴⁺ and is ascribed to [FeII(tpenaO)]²⁺, derived from an intramolecular O atom insertion into an Fe–tpena donor bond. Proposed ion pairs, ([Fe(tpena)OIPh]Cl)⁺ and ([Fe(tpena)OIPh]ClO₄)⁺, are more stable than native [Fe(tpena)OIPh]²⁺ ions, suggesting that halogen-bonding, as for the solution and solid states, operates also in the gas phase.

General information

State: Published
Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics, University of Southern Denmark, University of New South Wales
Authors: de Sousa, D. P. (Ekstern), Wegeberg, C. (Ekstern), Vad, M. S. (Ekstern), Mørup, S. (Intern), Frandsen, C. (Intern), Donald, W. A. (Ekstern), McKenzie, C. J. (Ekstern)
Number of pages: 12
Pages: 3810–3820
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Chemistry: A European Journal
Volume: 22
Heralded source of bright multi-mode mesoscopic sub-Poissonian light

In a direct detection scheme, we observed 7.8 dB of twin-beam squeezing for multi-mode two-color squeezed vacuum generated via parametric downconversion. Applying postselection, we conditionally prepared a sub-Poissonian state of light containing \(6.3 \times 10^5\) photons per pulse on the average with the Fano factor \(0.63 \pm 0.01\). The scheme can be considered as the heralded preparation of pulses with the mean energy varying between tens and hundreds of fJ and the uncertainty considerably below the shot-noise level. Such pulses can be used in metrology (for instance, for radiometer calibration), as well as for probing multi-mode non-linear optical effects. (C) 2016 Optical Society of America
Heterogeneous grain-scale response in ferroic polycrystals under electric field

Understanding coupling of ferroic properties over grain boundaries and within clusters of grains in polycrystalline materials is hindered due to a lack of direct experimental methods to probe the behaviour of individual grains in the bulk of a material. Here, a variant of three-dimensional X-ray diffraction (3D-XRD) is used to resolve the non-180° ferroelectric domain switching strain components of 191 grains from the bulk of a polycrystalline electro-ceramic that has undergone an electric-field-induced phase transformation. It is found that while the orientation of a given grain relative to the field direction has a significant influence on the phase and resultant domain texture, there are large deviations from the average behaviour at the grain scale. It is suggested that these deviations arise from local strain and electric field neighbourhoods being highly heterogeneous within the bulk polycrystal. Additionally, the minimisation of electrostatic potentials at the grain boundaries due to interacting ferroelectric domains must also be considered. It is found that the local grain-scale deviations average out over approximately 10–20 grains. These results provide unique insight into the grain-scale interactions of ferroic materials and will be of value for future efforts to comprehensively model these and related materials at that length-scale.

General information

State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, University of New South Wales, European Synchrotron Radiation Facility, Ulsan National Institute of Science and Technology
Authors: Daniels, J. E. (Ekstern), Majkut, M. (Intern), Cao, Q. (Ekstern), Schmidt, S. (Intern), Wright, J. (Ekstern), Jo, W. (Ekstern), Oddershede, J. (Intern)
High-definition velocity-space tomography of fast-ion dynamics

Velocity-space tomography of the fast-ion distribution function in a fusion plasma is usually a photon-starved tomography method due to limited optical access and signal-to-noise ratio of fast-ion Dα (FIDA) spectroscopy as well as the strive for high-resolution images. In high-definition tomography, prior information makes up for this lack of data. We restrict the target velocity space through the measured absence of FIDA light, impose phase-space densities to be non-negative, and encode the known geometry of neutral beam injection (NBI) sources. We further use a numerical simulation as prior information to reconstruct where in velocity space the measurements and the simulation disagree. This alternative approach is demonstrated for four-view as well as for two-view FIDA measurements. The high-definition tomography tools allow us to study fast ions in sawtoothing plasmas and the formation of NBI peaks at full, half and one-third energy by time-resolved tomographic movies.
Higher order mode optical fiber Raman amplifiers

We review higher order mode Raman amplifiers and discuss recent theoretical as well as experimental results including system demonstrations.

General information
State: Published
Organisations: Department of Photonics Engineering, Fiber Optics, Devices and Non-linear Effects, Centre of Excellence for Silicon Photonics for Optical Communications, Department of Physics
Authors: Rottwitt, K. (Intern), Friis, S. M. M. (Intern), Usuga Castaneda, M. A. (Intern), Christensen, E. N. (Intern), Koefoed, J. G. (Intern)
Number of pages: 4
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Series: International Conference on Transparent Optical Networks
ISSN: 2162-7339
Main Research Area: Technical/natural sciences
Conference: 18th International Conference on Transparent Optical Networks, Trento, Italy, 10/07/2016 - 10/07/2016

Higher order mode optical fiber Raman amplifiers

We review higher order mode Raman amplifiers and discuss recent theoretical as well as experimental results including system demonstrations.

General information
State: Published
Organisations: Department of Photonics Engineering, Fiber Optics, Devices and Non-linear Effects, Centre of Excellence for Silicon Photonics for Optical Communications, Department of Physics
Authors: Rottwitt, K. (Intern), Friis, S. M. M. (Intern), Usuga Castaneda, M. A. (Intern), Christensen, E. N. (Intern), Koefoed, J. G. (Intern)
Number of pages: 4
Publication date: 2016

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Title of host publication: Proceedings of 2016 18th International Conference on Transparent Optical Networks
Publisher: IEEE
Article number: Mo.D1.5
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Series: International Conference on Transparent Optical Networks
ISSN: 2162-7339
Main Research Area: Technical/natural sciences
Conference: 18th International Conference on Transparent Optical Networks, Trento, Italy, 10/07/2016 - 10/07/2016

High power microwave diagnostic for the fusion energy experiment ITER

Microwave diagnostics will play an increasingly important role in burning plasma fusion energy experiments like ITER and beyond. The Collective Thomson Scattering (CTS) diagnostic to be installed at ITER is an example of such a diagnostic with great potential in present and future experiments. The ITER CTS diagnostic will inject a 1 MW 60 GHz gyrotron beam...
into the ITER plasma and observe the scattering off fluctuations in the plasma — to monitor the dynamics of the fast ions
generated in the fusion reactions.

General information
State: Published
Organisations: Department of Physics, Plasma Physics and Fusion Energy, Center for Nuclear Technologies, Radiation
Physics, Universidade de Lisboa, Eindhoven University of Technology, Fusion For Energy
Authors: Korsholm, S. B. (Intern), Leipold, F. (Intern), Gonçalves, B. (Ekstern), Gutierrez Espinoza, H. E. (Intern), Jensen,
Nonbøl, E. (Intern), Oosterbeek, H. (Ekstern), Rasmussen, J. (Intern), Salewski, M. (Intern), Sanchez, P. (Ekstern),
Pedersen, M. S. (Intern), Taormina, A. (Intern)
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Series: International Conference on Infrared, Millimeter and Terahertz Waves
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Main Research Area: Technical/natural sciences
Conference: 41st International Conference on Infrared, Millimeter and Terahertz Waves, Copenhagen, Denmark,
Electronic versions:
IRMMW_synopsis_Korsholm_ITER_CTS_PID4361567.pdf
DOIs:
10.1109/IRMMW-THz.2016.7758537
Source: FindIt
Source-ID: 2349436767
Publication: Research - peer-review › Article in proceedings – Annual report year: 2016

High Power Microwave Diagnostic for the Fusion Energy Experiment ITER

General information
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Organisations: Department of Physics, Plasma Physics and Fusion Energy, Center for Nuclear Technologies, Radiation
Physics, Universidade de Lisboa, Eindhoven University of Technology, Fusion For Energy
Authors: Korsholm, S. B. (Intern), Leipold, F. (Intern), Gonçalves, B. (Ekstern), Gutierrez Espinoza, H. E. (Intern), Jensen,
Nonbøl, E. (Intern), Oosterbeek, H. (Ekstern), Rasmussen, J. (Intern), Salewski, M. (Intern), Sanchez, L. (Ekstern),
Sanchez, P. (Ekstern), Pedersen, M. S. (Intern), Taormina, A. (Intern)
Publication date: 2016
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Copenhagen, Denmark.
Main Research Area: Technical/natural sciences
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Source: PublicationPreSubmission
Source-ID: 127089775
Publication: Research - peer-review › Poster – Annual report year: 2016

How should we fuel future fusion power plants?

General information
State: Published
Organisations: Department of Physics, Plasma Physics and Fusion Energy
Authors: Thrysøe, A. S. (Intern), Madsen, J. (Intern), Naulin, V. (Intern), Nielsen, A. H. (Intern), Rasmussen, J. J. (Intern)
Number of pages: 1
Publication date: 2016
Main Research Area: Technical/natural sciences
Links:
http://www.sustain.dtu.dk/
H₂/D₂ exchange reaction on mono-disperse Pt clusters: enhanced activity from minute O₂ concentrations

The H₂/D₂ exchange reaction was studied on mono-disperse Pt8 clusters in a μ-reactor. The chemical activity was studied at temperatures varying from room temperature to 180 °C using mass spectrometry. It was found that minute amounts of O₂ in the gas stream increased the chemical activity significantly. XPS and ISS before and after reaction suggest little or no sintering during reaction. A reaction pathway is suggested based on DFT. H₂ desorption is identified as the rate-limiting step and O₂ is confirmed as the source of the increased activity. The binding energy of platinum atoms in a SiO₂ supported Pt₈ cluster is found to be comparable to the interatomic binding energies of bulk platinum, underlining the stability of the model system.
Hubbard-U corrected Hamiltonians for non-self-consistent random-phase approximation total-energy calculations: A study of ZnS, TiO$_2$, and NiO

In non-self-consistent calculations of the total energy within the random-phase approximation (RPA) for electronic correlation, it is necessary to choose a single-particle Hamiltonian whose solutions are used to construct the electronic density and noninteracting response function. Here we investigate the effect of including a Hubbard-U term in this single-particle Hamiltonian, to better describe the on-site correlation of 3d electrons in the transition-metal compounds ZnS, TiO$_2$, and NiO. We find that the RPA lattice constants are essentially independent of U, despite large changes in the underlying electronic structure. We further demonstrate that the non-selfconsistent RPA total energies of these materials have minima at nonzero U. Our RPA calculations find the rutile phase of TiO$_2$ to be more stable than anatase independent of U, a result which is consistent with experiments and qualitatively different from that found from calculations employing U-corrected (semi)local functionals. However we also find that the +U term cannot be used to correct the RPA’s poor description of the heat of formation of NiO.

General information
State: Published
Organisations: Department of Physics, Theoretical Atomic-scale Physics
Authors: Patrick, C. (Intern), Thygesen, K. S. (Intern)
Number of pages: 12
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- Scopus rating (2015): SJR 2.377 SNIP 1.13 CiteScore 2.8
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- 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
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- 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
Ammonia has been considered as a renewable and carbon free energy source. Aside from hydrogen, ammonia is the only carbon-free energy vector for transport application. As 26% of all CO$_2$ is emitted from transport sector, without reducing the emission from the transport sector, it will be impossible to significantly reduce overall CO$_2$ emission. Ammonia is the second most produced chemicals in the world. It has the lowest cost per GJ of energy among all the conventional fuels[1]. It has been described as an important chemical storage of hydrogen that can transform the world to a low-carbon economy. Ammonia can also be produced with no carbon footprint at all using e.g. wind or solar energy. The decentralized small scale ammonia production units developed by Reese et al. and Proton Ventures can be a good way to store electrical energy in liquid chemical. Even though ammonia cracking in combination with low temperature fuel cells have long term potential in automotive applications, in short-term, the most attractive option is direct ammonia combustion. Ammonia is also combusted to generate hydrogen via ammonia cracking and auto thermal reforming. However the challenges of homogeneous ammonia combustion are high ignition temperature, low combustion rate and N$_2$O and fuel NOx production. So, there is a need to develop new ammonia combustion system. One possible way to avoid these issues is catalytic combustion which has many advantages over conventional non-catalytic combustion, as ignition temperature is decreased and NOx emission is reduced because of the low operating temperature[11]. The combustion reaction is also easier to sustain for catalytic reaction.

In this study we present a bottom up approach to design a novel core-shell nanoparticulate catalyst of ruthenium (Ru) and copper (Cu). The CuRu catalyst invented in this work has proven to be superior in terms of catalytic activity towards ammonia oxidation compared to both copper and ruthenium. A systematic surface scientific investigation of thin films and supported nanoparticles have elucidated the reasoning behind activity enhancement.
Imaging ultrafast excited state pathways in transition metal complexes by X-ray transient absorption and scattering using X-ray free electron laser source

This report will describe our recent studies of transition metal complex structural dynamics on the fs and ps time scales using an X-ray free electron laser source, Linac Coherent Light Source (LCLS). Ultrafast XANES spectra at the Ni K-edge of nickel(ii) tetramesitylporphyrin (NiTMP) were measured for optically excited states at a timescale from 100 fs to 50 ps, providing insight into its sub-ps electronic and structural relaxation processes. Importantly, a transient reduced state Ni(i) (\(\text{tr}, 3d_{\text{x}_2-y_z}^{\text{occ}}\)) electronic state is captured through the interpretation of a short-lived excited state absorption on the low-energy shoulder of the edge, which is aided by the computation of X-ray transitions for postulated excited electronic states. The observed and computed inner shell to valence orbital transition energies demonstrate and quantify the influence of the electronic configuration on specific metal orbital energies. A strong influence of the valence orbital occupation on the inner shell orbital energies indicates that one should not use the transition energy from 1s to other orbitals to draw conclusions about the d-orbital energies. For photocatalysis, a transient electronic configuration could influence d-orbital energies up to a few eV and any attempt to steer the reaction pathway should account for this to ensure that external energies can be used optimally in driving desirable processes. NiTMP structural evolution and the influence of the porphyrin macrocycle conformation on relaxation kinetics can be likewise inferred from this study.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, SLAC National Accelerator Laboratory, Northwestern University, University of Washington, Argonne National Laboratory
Authors: Chen, L. X. (Ekstern), Shelby, M. L. (Ekstern), Lestrange, P. J. (Ekstern), Jackson, N. E. (Ekstern), Haldrup, K. (Intern), Mara, M. W. (Ekstern), Stickrath, A. B. (Ekstern), Zhu, D. (Ekstern), Lemke, H. (Ekstern), Chollet, M. (Ekstern), Hoffman, B. M. (Ekstern), Li, X. (Ekstern)
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Scopus rating (2017): SNIP 0.868 SJR 1.458 CiteScore 3.03
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BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.07 SJR 1.524 SNIP 0.903
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BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.489 SNIP 1.042 CiteScore 3.54
Web of Science (2015): Indexed yes
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Scopus rating (2014): SJR 1.732 SNIP 1.274 CiteScore 3.79
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BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.645 SNIP 1.149 CiteScore 3.65
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.751 SNIP 0.938 CiteScore 3.24
ISI indexed (2012): ISI indexed no
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.93 SNIP 1.232 CiteScore 3.92
ISI indexed (2011): ISI indexed no
BFI (2010): BFI-level 1
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.
Incorporation of a Cationic Conjugated Polyelectrolyte CPE within an Aqueous Poly(vinyl alcohol) Sol

We report on a multiscale polymer-within-polymer structure of the cationic conjugated polyelectrolyte poly([9,9-bis(6-N,N,N-trimethylammonium)hexyl]fluorene phenylene) (HTMAPFP) in aqueous poly(vinyl alcohol) (PVA) sol. Molecular dynamics simulations and small-angle neutron scattering (SANS) data show that HTMA-PFP forms aggregates in water but becomes entangled by PVA (with a 1:1 molar ratio of HTMA-PFP to PVA) and eventually immersed in PVA clusters (with the ratio 1:4). This is attributed to the hydrophobic hydrophilic balance. Contrast variation data with regular and deuterated PVA support a rigid body model, where HTMA-PFP is confined as locally isolated, but closely located, chains within PVA clusters, which alter correlation distances within the system. These results are supported by enhanced photoluminescence (PL) and ionic conductivity which, together with a red-shift in UV/vis absorption spectra, indicate the breakup of HTMA-PFP aggregates upon PVA addition.

General information
Inflow of atomic gas fuelling star formation

Gamma-ray burst host galaxies are deficient in molecular gas, and show anomalous metal-poor regions close to GRB positions. Using recent Australia Telescope Compact Array (ATCA) Hi observations we show that they have substantial atomic gas reservoirs. This suggests that star formation in these galaxies may be fuelled by recent inflow of metal-poor atomic gas. While this process is debated, it can happen in low-metallicity gas near the onset of star formation because gas cooling (necessary for star formation) is faster than the Hi-to-H$_2$ conversion.

General information
State: Published
Organisations: Department of Physics, Plasma Physics and Fusion Energy, University of Edinburgh, Universiteit Gent, University of Copenhagen, University of California at Santa Cruz, University of Leicester, Australia Telescope National Facility, University of Sydney, Aix Marseille Universite, Max-Planck-Institut fur extraterrestrische Physik, European Space Agency, Osservatorio Astronomico di Roma, Osservatorio Astrofisico Di Arcetri, Florence, Thüringer Landessternwarte Tautenburg, Laboratoire AIM-Paris-Saclay, National Institute for Astrophysics, University of Calabria, IT University of Copenhagen, Osservatorio Astronomico di Brera, Leiden University
Authors: Michałowski, M. J. (Ekstern), Gentile, G. (Ekstern), Hjorth, J. (Ekstern), Krumholz, M. R. (Ekstern), Tanvir, N. R. (Ekstern), Kamphuis, P. (Ekstern), Burlon, D. (Ekstern), Baes, M. (Ekstern), Basa, S. (Ekstern), Berta, S. (Ekstern), Castro Cerón, J. M. (Ekstern), Crosby, D. (Ekstern), D’Elia, V. (Ekstern), Elliott, J. (Ekstern), Greiner, J. (Ekstern), Hunt, L. K. (Ekstern), Klose, S. (Ekstern), Koprowski, M. P. (Ekstern), Le Floc’h, E. (Ekstern), Malesani, D. (Ekstern), Murphy, T. (Ekstern), Nicuesa Guelbenzu, A. (Ekstern), Palazzi, E. (Ekstern), Rasmussen, J. (Intern), Rossi, A. (Ekstern), Savaglio, S. (Ekstern), Schady, P. (Ekstern), De Ugarte Postigo, A. (Ekstern), Watson, D. (Ekstern), Van Der Werf, P. (Ekstern), Vergani, S. D. (Ekstern), Xu, D. (Ekstern)
Influence of gas atmospheres and ceria on the stability of nanoporous gold studied by environmental electron microscopy and \textit{in situ} ptychography

A novel complementary approach of electron microscopy/environmental TEM and \textit{in situ} hard X-ray ptychography was used to study the thermally induced coarsening of nanoporous gold under different atmospheres, pressures and after ceria deposition. The temperature applied during ptychographic imaging was determined by IR thermography. While using elevated temperatures (room temperature - 400 °C) and realistic gas atmospheres (1 bar) we achieved for the first time a spatial resolution of about 20 nm during hard X-ray ptychography. The annealing of pure and ceria stabilized nanoporous gold in different atmospheres revealed that the conditions have a tremendous influence on the coarsening. The porous structure of the samples was stable up to approximately 800 °C in vacuum, whereas pronounced changes and coarsening were observed already at approximately 300 °C in oxygen containing atmospheres. A layer of ceria on the nanoporous gold led to an improvement of the stability, but did not alleviate the influence of the gas atmosphere. Different behaviors were observed, such as coarsening and even material loss or migration. The results suggest that additional mechanisms beyond surface diffusion need to be considered and that microscopic studies aimed at more realistic conditions are important to understand the behavior of such materials and catalysts.

General information

State: Published
Organisations: Department of Physics, Center for Electron Nanoscopy, Center for Individual Nanoparticle Functionality, Paul Scherrer Institut, Karlsruhe Institute of Technology KIT, University of Bremen, Deutsches Elektronensynchrotron DESY
Authors: Baier, S. (Ekstern), Wittstock, A. (Ekstern), Damsgaard, C. D. (Intern), Diaz, A. (Ekstern), Reinhardt, J. (Ekstern), Benzi, F. (Ekstern), Shi, J. (Ekstern), Scherer, T. (Ekstern), Wang, D. (Ekstern), Kübel, C. (Ekstern), Schroer, C. G. (Ekstern), Grunwaldt, J. (Ekstern)
In Situ Ptychography of Heterogeneous Catalysts using Hard X-Rays: High Resolution Imaging at Ambient Pressure and Elevated Temperature

A new closed cell is presented for in situ X-ray ptychography which allows studies under gas flow and at elevated temperature. In order to gain complementary information by transmission and scanning electron microscopy, the cell makes use of a Protochips E-chip™ which contains a small, thin electron transparent window and allows heating. Two gold-based systems, 50 nm gold particles and nanoporous gold as a relevant catalyst sample, were used for studying the feasibility of the cell. Measurements showing a resolution around 40 nm have been achieved under a flow of synthetic air and during heating up to temperatures of 933 K. An elevated temperature exhibited little influence on image quality and resolution. With this study, the potential of in situ hard X-ray ptychography for investigating annealing processes of real catalyst samples is demonstrated. Furthermore, the possibility to use the same sample holder for ex situ electron microscopy before and after the in situ study underlines the unique possibilities available with this combination of electron microscopy and X-ray microscopy on the same sample.

General information
State: Published
Organisations: Center for Electron Nanoscopy, Experimental Surface and Nanomaterials Physics, Karlsruhe Institute of Technology KIT, Deutsches Elektronen-Synchrotron, Technische Universität Dresden, University of Bremen, European Synchrotron Radiation Facility
Integrating a dual-silicon photoelectrochemical cell into a redox flow battery for unassisted photocharging

Solar rechargeable flow cells (SRFCs) provide an attractive approach for in situ capture and storage of intermittent solar energy via photoelectrochemical regeneration of discharged redox species for electricity generation. However, overall SRFC performance is restricted by inefficient photoelectrochemical reactions. Here we report an efficient SRFC based on a dual-silicon photoelectrochemical cell and a quinone/bromine redox flow battery for in situ solar energy conversion and storage. Using narrow bandgap silicon for efficient photon collection and fast redox couples for rapid interface charge injection, our device shows an optimal solar-to-chemical conversion efficiency of similar to 5.9% and an overall photon-chemical-electricity energy conversion efficiency of similar to 3.2%, which, to our knowledge, outperforms previously reported SRFCs. The proposed SRFC can be self-photocharged to 0.8V and delivers a discharge capacity of 730 mAhr⁻¹. Our work may guide future designs for highly efficient solar rechargeable devices.

General information
State: Published
Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics, Department of Micro- and Nanotechnology, Silicon Microtechnology, Chinese Academy of Sciences
Authors: Liao, S. (Ekstern), Zong, X. (Ekstern), Seger, B. (Intern), Pedersen, T. (Intern), Yao, T. (Ekstern), Ding, C. (Ekstern), Shi, J. (Ekstern), Chen, J. (Ekstern), Li, C. (Ekstern)
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BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 11.8 SJR 6.414 SNIP 2.855
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 6.287 SNIP 2.86 CiteScore 11.23
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 6.41 SNIP 3.034 CiteScore 10.77
Web of Science (2014): Indexed yes
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Scopus rating (2013): SJR 6.206 SNIP 2.797 CiteScore 9.85
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Scopus rating (2012): SJR 5.866 SNIP 2.829 CiteScore 8.32
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
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ISI indexed (2011): ISI indexed no
Inter-ELM filamentary studies during density "shoulder" formation in ASDEX Upgrade

General information
State: Published
Organisations: Department of Physics, Plasma Physics and Fusion Energy, Josef Stefan Institute, University of Innsbruck, Max Planck Institute, Ecole Polytechnique Federale de Lausanne (EPFL), Consorzio RFX
Authors: Costea, S. (Ekstern), Carralero, D. (Ekstern), Madsen, J. (Intern), Vianello, N. (Ekstern), Naulin, V. (Intern), Nielsen, A. H. (Intern), Rasmussen, J. J. (Intern), Schrittwieser, R. (Ekstern), Ionita, C. (Ekstern), Spolaore, M. (Ekstern), Kovacic, J. (Ekstern)
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Intragranular orientation spread induced by grain interaction

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Organisations: Department of Mechanical Engineering, Materials and Surface Engineering, Department of Physics
Authors: Winther, G. (Intern), Oddershede, J. (Intern)
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Event: Abstract from TMS 2016 145th ANNUAL MEETING & EXHIBITION, Nashville, United States.
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Relations
Activities:
Intragranular orientation spread induced by grain interaction
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2017

Inversion methods for fast-ion velocity-space tomography in fusion plasmas

Velocity-space tomography has been used to infer 2D fast-ion velocity distribution functions. Here we compare the performance of five different tomographic inversion methods: truncated singular value decomposition, maximum entropy, minimum Fisher information and zeroth and first-order Tikhonov regularization. The inversion methods are applied to fast-ion Dα measurements taken just before and just after a sawtooth crash in the ASDEX Upgrade tokamak as well as to synthetic measurements from different test distributions. We find that the methods regularizing by penalizing steep gradients or maximizing entropy perform best. We assess the uncertainty of the calculated inversions taking into account photon noise, uncertainties in the forward model as well as uncertainties introduced by the regularization which allows us to distinguish regions of high and low confidence in the tomographies. In high confidence regions, all methods agree that ions with pitch values close to zero, as well as ions with large pitch values, are ejected from the plasma center by the sawtooth crash, and that this ejection depletes the ion population with large pitch values more strongly.

General information
State: Published
Organisations: Department of Physics, Plasma Physics and Fusion Energy, Max Planck Institute for Plasma Physics, University of California, Irvine
Authors: Jacobsen, A. S. (Intern), Stagner, L. (Ekstern), Salewski, M. (Intern), Geiger, B. (Ekstern), Heidbrink, W. (Ekstern), Korsholm, S. B. (Intern), Leipold, F. (Intern), Nielsen, S. K. (Intern), Rasmussen, J. (Intern), Pedersen, M. S. (Intern), Thomsen, H. (Ekstern), Weiland, M. (Ekstern)
Gd modified Pt(111) single crystals have been prepared in an ultra high vacuum (UHV). By vacuum deposition of ∼200 Å Gd on a sample heated to 800 °C, a Pt5Gd alloy terminated by a single atomic layer of Pt was formed. Subsequently the surfaces were characterized using low energy electron diffraction (LEED), showing that a highly ordered crystal structure had appeared. To study the molecular dynamics on this surface a detailed study of the CO adsorption on the surface was conducted using temperature programmed desorption (TPD) of CO. The TPD spectra show a desorption peak shifted down in temperature compared to those of pure Pt(111). The shape of the desorption peak and the desorption temperature were shown to be strongly dependent on the CO coverage of the surface. A systematic investigation of CO desorption temperature as a function of coverage was consequently performed. A simple simulation of the TPD spectra was carried out, based on adsorption energies from density functional theory (DFT). This simulation reproduces the shift and the narrowing of the desorption spectrum from the experiments and the DFT calculations suggest that the sharp TPD feature arises from cooperative adsorbate interactions, caused by subtle reconstructions occurring at coverages above 1/3 ML CO, whereas the overall temperature shift relative to pure Pt(111) comes from weaker CO binding due to the contraction of the Gd/Pt(111) surface.
Investigation of CO₂ reduction products on mass selected Cu nanoparticles

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Department of Physics, Experimental Surface and Nanomaterials Physics
Authors: Hogg, T. V. (Intern), Bertheussen, E. (Intern), Bodin, A. (Intern), Stephens, I. (Intern), Chorkendorff, I. (Intern)
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Main Research Area: Technical/natural sciences
Links: http://www.sustain.dtu.dk/
Investigation of noise sources in upconversion based infrared hyperspectral imaging
Noise sources in infrared hyperspectral imaging based on nonlinear frequency upconversion are investigated. The effects on the spectral and spatial content of the images are evaluated and methods of combating them are suggested.

Iso-acoustic focusing of cells for size-insensitive acousto-mechanical phenotyping
Mechanical phenotyping of single cells is an emerging tool for cell classification, enabling assessment of effective parameters relating to cells' interior molecular content and structure. Here, we present iso-acoustic focusing, an equilibrium method to analyze the effective acoustic impedance of single cells in continuous flow. While flowing through a microchannel, cells migrate sideways, influenced by an acoustic field, into streams of increasing acoustic impedance, until reaching their cell-type specific point of zero acoustic contrast. We establish an experimental procedure and provide theoretical justifications and models for iso-acoustic focusing. We describe a method for providing a suitable acoustic contrast gradient in a cell-friendly medium, and use acoustic forces to maintain that gradient in the presence of destabilizing forces. Applying this method we demonstrate iso-acoustic focusing of cell lines and leukocytes, showing that acoustic properties provide phenotypic information independent of size.
ITER perspective on fusion reactor diagnostics - A spectroscopic view
The ITER tokamak requires diagnostics that on the one hand have a high sensitivity, high spatial and temporal resolution and a high dynamic range, while on the other hand are robust enough to survive in a harsh environment. In recent years significant progress has been made in addressing critical challenges to the development of spectroscopic (but also other) diagnostics. This contribution presents an overview of recent achievements in 4 topical areas: First mirror protection and cleaning, Nuclear confinement, Radiation mitigation strategy for optical and electronic components and Calibration strategies.
Keeping things open
This year we are celebrating the 100th anniversary of the papers by Niels Bohr introducing the atomic model that dominated twentieth century physics. Niels Bohr himself remained an influential participant in the development for almost 50 years, and his institute became a magnet for young researchers and an important center for the development of modern physics. From both a personal and a scientific perspective – being both a grandson of Niels Bohr and a physicist – I shall try to assess some of the characteristics of Bohr’s personality and his approach to science that made this possible.
Key role of internal electric fields in the properties of ionic materials containing transition-metal complexes

Layered Surface Detection in Micro-CT Tetra Pak Data

L-H power threshold studies with tungsten/carbon divertor on the EAST tokamak
threshold is observed in EAST with the tungsten/carbon divertor, compared to the carbon divertor after intensive lithium wall coating. A newly installed cryopump increasing the pumping efficiency also plays an important part in the observed lower threshold. In addition, the H-mode in the Quasi-Snowflake divertor configuration has been obtained on EAST, exhibiting higher L-H power threshold compared to the lower single null configuration with similar $I_p/B_T$ pairs.

**General information**

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Organisations: Department of Physics, Plasma Physics and Fusion Energy, Chinese Academy of Sciences
Authors: Chen, L. (Ekstern), Xu, G. S. (Ekstern), Gao, W. (Ekstern), Zhang, L. (Ekstern), Nielsen, A. H. (Intern), Luo, Z. P. (Ekstern), Si, H. (Ekstern), Wang, Y. M. (Ekstern), Qu, H. (Ekstern), Sun, Z. (Ekstern), Duan, Y. M. (Ekstern), Liu, H. Q. (Ekstern), Wang, S. X. (Ekstern), Li, M. H. (Ekstern), Zhang, X. J. (Ekstern), Wu, B. (Ekstern), Chen, R. (Ekstern), Wang, L. (Ekstern), Wang, H. Q. (Ekstern), Ding, S. Y. (Ekstern), Yan, N. (Ekstern), Liu, S. C. (Ekstern), Shao, L. M. (Ekstern), Zhang, W. (Ekstern), Hu, G. H. (Ekstern), Li, J. (Ekstern), Li, Y. L. (Ekstern), Wu, X. Q. (Ekstern), Zhao, N. (Ekstern), Jia, M. N. (Ekstern)
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Web of Science (2017): Indexed Yes
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Scopus rating (2016): SJR 0.209 SNIP 0.445 CiteScore 0.45
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.226 SNIP 0.486 CiteScore 0.47
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.244 SNIP 0.412 CiteScore 0.5
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.297 SNIP 0.571 CiteScore 0.56
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.259 SNIP 0.402 CiteScore 0.48
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.254 SNIP 0.484 CiteScore 0.45
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.395 SNIP 0.621
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.308 SNIP 0.553
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.268 SNIP 0.555
Scopus rating (2007): SJR 0.218 SNIP 0.558
Scopus rating (2006): SJR 0.32 SNIP 0.615
Scopus rating (2005): SJR 0.3 SNIP 0.566
Scopus rating (2004): SJR 0.303 SNIP 0.36
Scopus rating (2003): SJR 0.293 SNIP 0.516
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: 2AV.2.34_PVSEC_M._Plakhotnyuk_poster.pdf

Relations
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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 nano-structures 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.

General information
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Organisations: Department of Micro- and Nanotechnology, Silicon Microtechnology, Nanoprobes, Department of Photonics Engineering, Plasmonics and Metamaterials, Department of Energy Conversion and Storage, Fundamental Electrochemistry, Experimental Surface and Nanomaterials Physics
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Host publication Information
Light-matter interaction in low-dimensional materials. A theoretical study
In this thesis we have investigated the optical properties of layered and two-dimensional materials for application in the field of plasmonics and metamaterials using Density Functional Theory (DFT). Both of these fields, if successful in their goals, promise new technologies for small scale photonics beyond the diffraction limit. A technological breakthrough of such a caliber would have far reaching consequences such as enabling a practical interface to nano scale integrated electronic circuits or enable the construction of novel devices like a superlens with resolution well beyond diffraction limit. However, the progress of these fields is currently inhibited by large losses that can only be resolved through the discovery of new materials.

Using linear response time-dependent DFT we calculate the optical properties of several experimentally known layered transition metal dichalcogenides (TMDs) with the chemical formula of MX2 where M is a transition metal and X is a chalcogen atom (S, Se, Te). The TMDs constitute an interesting class of materials due to their diverse range of properties including both metals and semi-conductors. We find that the TMDs with group 5 transition metal atoms in the H monolayer exhibit a special bandstructure in which metallic bands are separated from other valence and conduction bands by finite energy gaps which has the potential to minimize the optical losses by reducing the density of states for scattering. The size of the energy gaps are, however, not sufficiently large to completely eliminate optical losses. We therefore propose a new class of layered materials with the chemical formula 2H-MXY where M is a group 4 transition metal atom, X is a chalcogen atom, and Y is a halogen atom (Cl, Br, I) which increases the size of the energy gaps and significantly reduces optical losses. This entails improved plasmonic normalized propagation lengths and superior lifetimes compared to the best plasmonic material, namely, silver.

We show that all of the TMDs are natural hyperbolic materials, which means that they exhibit a strongly anisotropic dielectric response reflected by a sign-difference in their dielectric tensor resulting in hyperbolic isofrequency contours. Hyperbolic metamaterials obtain their anisotropic response from an artificial sub-wavelength structuring and are limited in their performance by the period of the structuring - the smaller, the better. In contrast, natural hyperbolic materials suffer no such limitation due to their lack of artificial structuring, and indeed, we find a much greater performance for all applications of hyperbolic materials.

The possibility of stacking individual two-dimensional materials into so-called van der Waals heterostructures is perhaps one of the most interesting technological developments in the field of two-dimensional materials. We show that effective medium theory for the dielectric properties of graphene and hexagonal boron nitride heterostructures, which treat the heterostructure as a continuous medium, break down for atomically thin layers due to quantum mechanical effects but also for thick components due to multiple reflection effects. We propose an extended version of effective medium theory to account for the interface layers and show that the effective medium description is improved.

The determination of the quality of materials for application within plasmonics and metamaterials requires an accurate calculation of the optical properties of materials which can be computationally demanding. To reduce the computational costs, the linear tetrahedron method and the employment of symmetries have been implemented which in some cases can reduce the computational costs by a factor of 200.
Limitations of effective medium theory in multilayer graphite/hBN heterostructures

We apply effective medium theory (EMT) to metamaterials consisting of a varying number of consecutive sheets of graphene and hexagonal boron nitride, and compare this with a full calculation of the permittivity and the reflection based on the tight binding method and the transfer matrix method in order to study the convergence to EMT. We find that convergence is reached for both in-plane and out-of-plane directions already for five sheets but that for ≈30 sheets multiple reflection effects causes the reflection spectrum to differ from EMT. We show that modes that are evanescent in air are extremely sensitive to the electronic details of the sheets near the structure boundary and that EMT estimates poorly the reflection of these modes, causing an overestimation of the Purcell factor. Finally, we offer an improved EMT, which gives far better convergence in the low-energy regime.
Low-to-high confinement transition mediated by turbulence radial wave number spectral shift in a fusion plasma

A new model for the low-to-high (L-H) confinement transition has been developed based on a new paradigm for turbulence suppression by velocity shear [G. M. Staebler et al., Phys. Rev. Lett.110, 055003 (2013)]. The model indicates that the L-H transition can be mediated by a shift in the radial wave number spectrum of turbulence, as evidenced here, for the first time, by the direct observation of a turbulence radial wave number spectral shift and turbulence structure tilting prior to the L-H transition at tokamak edge by direct probing. This new mechanism does not require a pretransition overshoot in the turbulent Reynolds stress, shunting turbulence energy to zonal flows for turbulence suppression as demonstrated in the experiment.

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Magnetic field controlled charge density wave coupling in underdoped YBa$_2$Cu$_3$O$_{6+x}$

The application of magnetic fields to layered cuprates suppresses their high-temperature superconducting behaviour and reveals competing ground states. In widely studied underdoped YBa$_2$Cu$_3$O$_{6+x}$ (YBCO), the microscopic nature of field-
induced electronic and structural changes at low temperatures remains unclear. Here we report an X-ray study of the high-field charge density wave (CDW) in YBCO. For hole dopings $\sim 0.123$, we find that a field ($B \sim 10$ T) induces additional CDW correlations along the CuO chain ($b$-direction) only, leading to a three-dimensional (3D) ordered state along this direction at $B \sim 15$ T. The CDW signal along the $a$-direction is also enhanced by field, but does not develop an additional pattern of correlations. Magnetic field modifies the coupling between the CuO$_2$ bilayers in the YBCO structure, and causes the sudden appearance of the 3D CDW order. The mirror symmetry of individual bilayers is broken by the CDW at low and high fields, allowing Fermi surface reconstruction, as recently suggested.
Making the most of materials computations

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Mapping of strain mechanisms in barium titanate by three-dimensional X-ray diffraction

This thesis presents an in-situ three-dimensional study of the grain-scale response of a prototypical piezoelectric ceramic, barium titanate (BT), to an externally applied electric field. Piezoceramics take advantage of the coupling of electrical and mechanical energies for use in sensors and actuators, found in both common applications such as fuel injectors and specialized applications such as medical imaging equipment. Since piezoceramics are typically used in the polycrystalline state it is important to consider not just the crystal structure but also the role of intergranular effects in the structure-properties relationships. Such effects are difficult to observe using destructive two-dimensional microscopy techniques and averaged over the entire sample in conventional powder diffraction studies. We instead use a combination of nondestructive three-dimensional X-ray diffraction techniques to study the material at the grain scale.

First, we use the intensity ratios of split diffraction peaks to extract grain-scale domain volume fractions for 139 grains. We find that even in the as-processed state there exist unequal volume fractions of each domain type, which we attribute to a heterogeneous local environment at the cubic to tetragonal transition during processing. When a field is applied, we observe a first-order orientation dependence with second order deviations, again attributed to the grain neighbourhood effect. Corellation of this with microstructural parameters such as grain size, neighbour misorientation and position within the sample did not reveal any obvious causes.

Next we develop a novel indexing and refinement method whereby the peak positions of domains are forward projected from crystallographic twinning orientations and the deviation between projected and measured diffraction patterns is minimized to refine domain-scale orientations and lattice parameters. We present the results of refinement for a bulk grain in which the domains are found to be misoriented from perfect crystallographic twins by 0.1-0.3°, suggesting a strained microstructure. The data set was collected by illuminating the entire width of the sample with a box beam, thus it contains a statistically significant number of grains for which domain-scale parameters will be refined in the future.
Material transfer in Pulsed Laser Deposition of the solar cell materials Cu$_2$SnS$_3$ and Cu$_2$ZnSnS$_4$.

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Maximising electro-mechanical response by minimising grain-scale strain heterogeneity in phase-change actuator ceramics
Phase-change actuator ceramics directly couple electrical and mechanical energies through an electric-field-induced phase transformation. These materials are promising for the replacement of the most common electro-mechanical ceramic, lead zirconate titanate, which has environmental concerns. Here, we show that by compositional modification, we reduce the grain-scale heterogeneity of the electro-mechanical response by 40%. In the materials investigated, this leads to an increase in the achievable electric-field-induced strain of the bulk ceramic of 45%. Compositions of (100-x)Bi$_{0.5}$Na$_{0.5}$TiO$_3$-(x)BaTiO$_3$, which initially possess a pseudo-cubic symmetry, can be tuned to undergo phase transformations to combined lower symmetry phases, thus decreasing the anisotropy of the transformation strain. Further, modelling of transformation strains of individual grains shows that minimum grain-scale strain heterogeneity can be achieved by precise control of the lattice distortions and orientation distributions of the induced phases. The current results can be used to guide the design of next generation high-strain electro-mechanical ceramic actuator materials.

General information
State: Published
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Maximum modulation of plasmon-guided modes by graphene gating

The potential of graphene in plasmonic electro-optical waveguide modulators has been investigated in detail by finite-element method modelling of various widely used plasmonic waveguiding configurations. We estimated the maximum possible modulation depth values one can achieve with plasmonic devices operating at telecom wavelengths and exploiting the optical Pauli blocking effect in graphene. Conclusions and guidelines for optimization of modulation/intrinsic loss trade-off have been provided and generalized for any graphene-based plasmonic waveguide modulators, which should help in consideration and design of novel active-plasmonic devices.
mBEEF-vdW: Robust fitting of error estimation density functionals

We propose a general-purpose semilocal/nonlocal exchange-correlation functional approximation, named mBEEF-vdW. The exchange is a meta generalized gradient approximation, and the correlation is a semiflocal and nonlocal mixture, with the Rutgers-Chalmers approximation for van der Waals (vdW) forces. The functional is fitted within the Bayesian error estimation functional (BEEF) framework [J. Wellendorff et al., Phys. Rev. B 85, 235149 (2012); J. Wellendorff et al., J. Chem. Phys. 140, 144107 (2014)]. We improve the previously used fitting procedures by introducing a robust MM-estimator based loss function, reducing the sensitivity to outliers in the datasets. To more reliably determine the optimal model complexity, we furthermore introduce a generalization of the bootstrap 0.632 estimator with hierarchical bootstrap sampling and geometric mean estimator over the training datasets. Using this estimator, we show that the robust loss function leads to a 10% improvement in the estimated prediction error over the previously used least-squares loss function. The mBEEF-vdW functional is benchmarked against popular density functional approximations over a wide range of datasets relevant for heterogeneous catalysis, including datasets that were not used for its training. Overall, we find that mBEEF-vdW has a higher general accuracy than competing popular functionals, and it is one of the best performing functionals on chemisorption systems, surface energies, lattice constants, and dispersion. We also show the potential-energy curve of graphene on the nickel(111) surface, where mBEEF-vdW matches the experimental binding length. mBEEF-vdW is currently available in GPAW and other density functional theory codes through Libxc, version 3.0.0.
Measurement-Induced Macroscopic Superposition States in Cavity Optomechanics

A novel protocol for generating quantum superpositions of macroscopically distinct states of a bulk mechanical oscillator is proposed, compatible with existing optomechanical devices operating in the bad-cavity limit. By combining a pulsed optomechanical quantum nondemolition (QND) interaction with nonclassical optical resources and measurement-induced feedback, the need for strong single-photon coupling is avoided. We outline a three-pulse sequence of QND interactions encompassing squeezing-enhanced cooling by measurement, state preparation, and tomography.

General information
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BFI (2011): BFI-level 2
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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
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Scopus rating (2008): SJR 6.194 SNIP 2.837
Web of Science (2008): Indexed yes
Mesoscopic current transport in two-dimensional materials with grain boundaries: Four-point probe resistance and Hall effect
We have studied the behavior of micro four-point probe (M4PP) measurements on two-dimensional (2D) sheets composed of grains of varying size and grain boundary resistivity by Monte Carlo based finite element (FE) modelling. The 2D sheet of the FE model was constructed using Voronoi tessellation to emulate a polycrystalline sheet, and a square sample was cut from the tessellated surface. Four-point resistances and Hall effect signals were calculated for a probe placed in the center of the square sample as a function of grain density $n$ and grain boundary resistivity $\rho_{GB}$. We find that the dual configuration sheet resistance as well as the resistance measured between opposing edges of the square sample have a simple unique dependency on the dimensionless parameter $\sqrt{n\rho_{GB}G_0}$, where $G_0$ is the sheet conductance of a grain. The value of the ratio $R_A/R_B$ between resistances measured in A- and B-configurations depends on the dimensionality of the current transport (i.e., one- or two-dimensional). At low grain density or low grain boundary resistivity, two-dimensional transport is observed. In contrast, at moderate grain density and high grain resistivity, one-dimensional transport is seen. Ultimately, this affects how measurements on defective systems should be interpreted in order to extract relevant sample parameters. The Hall effect response in all M4PP configurations was only significant for moderate grain densities and fairly large grain boundary resistivity.

**General information**

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Organisations: Department of Micro- and Nanotechnology, Department of Physics, Quantum Physics and Information Technology, Silicon Microtechnology, Center for Individual Nanoparticle Functionality
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Metallization of cyanide-modified Pt(111) electrodes with copper

The reduction of Cu$^{2+}$ ions irreversibly attached to the surface of a cyanide-modified Pt(111) electrode via non-covalent or weakly covalent interactions with the N atom of adsorbed cyanide was studied using cyclic voltammetry (CV) and in situ scanning tunneling microscopy (STM). Both CV and STM provide evidence that the reduction of irreversibly adsorbed Cu$^{2+}$ to Cu in Cu$^{2+}$-free sulfuric acid solutions does not result in the stripping of the cyanide adlayer. This strongly suggests that the reduction process results in the metallization of the cyanide adlayer on Pt(111), yielding a platinum-cyanide-copper sandwich configuration. STM also shows that the Cu deposit consists of isolated bidimensional nanoislands, which slowly grow through an Ostwald ripening mechanism if the potential is kept negative of the reduction peak. Metallization is not possible in perchloric acid solutions, which implies that the specific adsorption of sulfate on the bidimensional Cu nanoislands plays an important role in stabilizing them. This was confirmed by the observation on the nanoislands, using in situ STM, of the structure typical for adsorbed sulfate on the (111) faces of fcc.
Microfluidics of sugar transport in plant leaves and in biomimetic devices

The physical mechanisms underlying vital plant functions constitute a research field with many important, unsolved problems. Some of these research topics gaining attention in recent years are concerned with the fluid transport in plants. Plants photosynthesize sugars in their leaves for energy production and growth. These sugars are taken up into the veins of the leaf and then transported efficiently to other parts of the plant via the vascular system. The vascular system of plants has two types of tissue: the xylem brings water from the roots up to the leaves, and the phloem transports sugars from the sources in the leaves to the sinks in roots, fruits and regions of growth. The transport of sugar solution in the phloem is driven by an osmotic pumping mechanism. The uptake of water from the xylem into the phloem generates a hydrostatic pressure difference between sources and sinks which results in a bulk flow of sugar solution. It is not clear where in the leaf this bulk flow starts, especially in plants that have intercellular connections (plasmodesmata) between the phloem and the cells surrounding the veins. In these plants bulk flow could be involved in the process of sugar loading into the veins.

We studied the physics of two basic mechanisms for sugar loading: the polymer trap and passive loading. The polymer trap is an active mechanism, which is characterized by an elevated concentration of sugars inside the veins compared to the rest of the leaf. This is achieved with the help of enzymes combining sucrose molecules entering the vein through plasmodesmata into larger sugar molecules. These molecules are then too large to move back out of the vein. In order for this system to work, the plasmodesmata have to act as extremely precise filters. Microscopy studies show that these plasmodesmata are very small, in fact they are too small to resolve their exact cross section available to transport. In our theoretical model, we approximated the plasmodesmata as cylindrical slit pores and investigated whether the pores could be small enough to fulfill the filtering function, and at the same time large enough to allow for sufficient transport of sucrose. We found that this mechanism is indeed feasible. We could further conclude that sugar is not only transported by diffusion, but is partly advected through the plasmodesmata by a bulk flow. This bulk flow is actually enough to drive the export from the leaf, meaning that no additional water has to be taken up into the phloem in order to drive the flow.

In plants that use passive loading instead, the concentration of sugars inside the veins is lower than in the surrounding tissue, and the plasmodesmata connecting the phloem with the cells surrounding the veins are larger than in the polymer trap case. We suspected, that in passive loading the advective transport contribution to sugar loading could be even more important than in the polymer trap. We demonstrated advective loading of sugars in experiments with biomimetic devices, modeling the leaf as a system of three compartments: phloem, xylem and sugar producing tissue. We further developed a theoretical model of passive loading, enabling us to identify the key parameters that determine the sugar uptake into the phloem. Assuming values typically found in plants for the three key parameters sugar concentration, interface areas between the three compartments and pore size of the plasmodesmata, the uptake of sugar can be dominated by either advection or diffusion. Of these key parameters, the pore size has the largest influence on the ratio of advective to diffusive loading. The next step in the transport of sugars is the export from the leaf. We studied the case of conifer needles, which are linear leaves with unbranched venation. Most conifer leaves are not longer than 6 cm, which is rather short compared to broad leaves with sizes spanning from millimeters to meters. In order to understand this limitation we modeled the phloem conduits in linear leaves as cylindrical, osmotic pipes running from the tip to the base of the needle. Using a simple analytical model we calculated the sugar export rate from these conduits assuming a constant concentration of sugars along the pipe. We found that in needles longer than a characteristic length the fluid close to the tip becomes stagnant and sugars can no longer be exported efficiently. This means, that very little output can be gained from making a leaf longer than the efficient leaf length. Our prediction for an efficient leaf length matches well with the mean needle lengths from a data set comprising 519 of the 629 currently known conifer species.

We further calculated the energy dissipated by the export of sugar solution from linear osmotic pipes. There are two main contributions to the dissipation of energy, one due to the resistance of membrane pores and one due to Poiseuille resistance inside the pipe. We found simple and general analytical solutions for flow rates and dissipation of energy for single pipes, generalizing the normal Poiseuille expression and showing that the driving force is not only the pressure, but the “water potential”, which is a combination of concentration and pressure. We also treated a system of coupled parallel pipes with a power law distribution of lengths, as found in linear leaves. The results for the system of coupled pipes are surprisingly similar to the single pipe solutions, and likewise show the emergence of the stagnant zone for leaves longer than the effective length.

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Relations
Mid-infrared nonlinear upconversion imaging and sensing

The mid-IR wavelength range is highly relevant for a number of applications related to gas spectroscopy and spectral analysis of complex molecules such as those including CH bounds. The main obstacles for exploitation of mid-IR applications include suitable and affordable mid-IR light sources for excitation of the sample and sensitive mid-IR detectors. With the advent of mid-IR Quantum cascaded lasers and super continuum light sources new possibilities has emerged. However, low-noise, mid-IR (2-15 μm) detection is still challenging requiring cryogenic cooling to gain sensitivities needed for measurements of fluorescence or absorptions signals. Mid-IR upconversion imaging and detection using nonlinear crystals offers good promise as an alternative, sensitive mid-IR imaging and detection technology. In this paper the fundamental properties of upconversion is discussed.

Mid-infrared upconversion spectroscopy

Mid-infrared (MIR) spectroscopy is emerging as an attractive alternative to near-infrared or visible spectroscopy. MIR spectroscopy offers a unique possibility to probe the fundamental absorption bands of a large number of gases as well as the vibrational spectra of complex molecules. In this paper we discuss non-collinear upconversion as a means for obtaining MIR spectra in the 5-10 μm range with a resolution better than 20 cm⁻¹ over the full interval using four discrete phase-match settings. A theoretical treatment of non-collinear upconversion is given and two different experimental implementations are tested.
Millimeter-wave receiver design for plasma diagnostics
Scattered millimeter waves entering from the collective Thomson scattering diagnostic at ASDEX Upgrade fusion device are generally elliptically polarized. In order to convert the millimeter waves to linearly polarized waves (required for the detector), birefringent window assemblies (sapphire) have been developed to replace grooved metal mirrors. This allows a significantly more compact receiver design which is less susceptible to misalignment. The setup has been tested and implemented at ASDEX Upgrade.

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Modeling of microdevices for SAW-based acoustophoresis - A study of boundary conditions
We present a finite-element method modeling of acoustophoretic devices consisting of a single, long, straight, water-filled microchannel surrounded by an elastic wall of either borosilicate glass (pyrex) or the elastomer polydimethylsiloxane (PDMS) and placed on top of a piezoelectric transducer that actuates the device by surface acoustic waves (SAW). We compare the resulting acoustic fields in these full solid-fluid models with those obtained in reduced fluid models comprising only a water domain with simplified, approximate boundary conditions representing the surrounding solids. The reduced models are found to only approximate the acoustically hard pyrex systems to a limited degree for large wall thicknesses and but not very well for acoustically soft PDMS systems shorter than the PDMS damping length of 3 mm.

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Organisations: Department of Physics, Biophysics and Fluids
Authors: Skov, N. R. (Intern), Bruus, H. (Intern)
Number of pages: 14
Modelling third harmonic ion cyclotron acceleration of deuterium beams for JET fusion product studies experiments

Recent JET experiments have been dedicated to the studies of fusion reactions between deuterium (D) and Helium-3 (³He) ions using neutral beam injection (NBI) in synergy with third harmonic ion cyclotron radio-frequency heating (ICRH) of the beam. This scenario generates a fast ion deuterium tail enhancing DD and D³He fusion reactions. Modelling and measuring the fast deuterium tail accurately is essential for quantifying the fusion products. This paper presents the modelling of the D distribution function resulting from the NBI+ICRF heating scheme, reinforced by a comparison with dedicated JET fast ion diagnostics, showing an overall good agreement. Finally, a sawtooth activity for these experiments has been observed and interpreted using SPOT/RFOF simulations in the framework of Porcelli’s theoretical model, where NBI+ICRH accelerated ions are found to have a strong stabilizing effect, leading to monster sawteeth.

General information

State: Published
Organisations: Department of Physics, Plasma Physics and Fusion Energy, Institute for Magnetic Fusion Research, KTH - Royal Institute of Technology, Uppsala University, European Commission, Istituto di Fisica del Plasma, Abraham F. Ioffe Institute, Culham Science Centre, Aalto University, Catalan Institution for Research and Advanced Studies, Università degli Studi di Milano-Bicocca
Authors: Schneider, M. (Ekstern), Johnson, T. (Ekstern), Dumont, R. (Ekstern), Eriksson, J. (Ekstern), Eriksson, L. (Ekstern), Giacomelli, L. (Ekstern), Girardo, J. (Ekstern), Hellsten, T. (Ekstern), Khilkevitch, E. (Ekstern), Kiptily, V. (Ekstern), Koskela, T. (Ekstern), Mansinen, M. (Ekstern), Novcet, M. (Ekstern), Salewski, M. (Intern), Sharapov, S. (Ekstern), Shevelev, A. (Ekstern)
Number of pages: 16
Publication date: 2016
Main Research Area: Technical/natural sciences
Multi-code analysis of scrape-off layer filament dynamics in MAST

Four numerical codes are employed to investigate the dynamics of scrape-off layer filaments in tokamak relevant conditions. Experimental measurements were taken in the MAST device using visual camera imaging, which allows the evaluation of the perpendicular size and velocity of the filaments, as well as the combination of density and temperature associated with the perturbation. A new algorithm based on the light emission integrated along the field lines associated with the position of the filament is developed to ensure that it is properly detected and tracked. The filaments are found to have velocities of the order of 1 km s\(^{-1}\), a perpendicular diameter of around 2-3 cm and a density amplitude 2-3.5 times the background plasma. 3D and 2D numerical codes (the STORM module of BOUT++, GBS, HESEL and TOKAM3X) are used to reproduce the motion of the observed filaments with the purpose of validating the codes and of better understanding the experimental data. Good agreement is found between the 3D codes. The seeded filament simulations are also able to reproduce the dynamics observed in experiments with accuracy up to the experimental errorbar levels. In addition, the numerical results showed that filaments characterised by similar size and light emission intensity can have quite different dynamics if the pressure perturbation is distributed differently between density and temperature components. As an additional benefit, several observations on the dynamics of the filaments in the presence of evolving temperature fields were made and led to a better understanding of the behaviour of these coherent structures.
Multi-electrode probe geometry optimization for characterization of magnetic tunnel junction stacks

General information
State: Published
Organisations: Center for Nanostructured Graphene, Department of Micro- and Nanotechnology, Silicon Microtechnology, Experimental Surface and Nanomaterials Physics, Nanocarbon
Authors: Cagliani, A. (Intern), Kjær, D. (Intern), Østerberg, F. W. (Intern), Hansen, O. (Intern), Nielsen, P. F. (Intern), Petersen, D. H. (Intern)
Number of pages: 1
Multigrain indexing of unknown multiphase materials

A multigrain indexing algorithm for use with samples comprising an arbitrary number of known or unknown phases is presented. No a priori crystallographic knowledge is required. The algorithm applies to data acquired with a monochromatic beam and a conventional two-dimensional detector for diffraction. Initially, candidate grains are found by searching for crystallographic planes, using a Dirac comb convoluted with a box function as a filter. Next, candidate grains are validated and the unit cell is optimized. The algorithm is validated by simulations. Simulations of 500 cementite grains and similar to 100 reflections per grain resulted in 99.2% of all grains being indexed correctly and 99.5% of the reflections becoming associated with the right grain. Simulations with 200 grains associated with four mineral phases and 50-700 reflections per grain resulted in 99.9% of all grains being indexed correctly and 99.9% of the reflections becoming associated with the right grain. The main limitation is in terms of overlap of diffraction spots and computing time. Potential areas of use include three-dimensional grain mapping, structural solution and refinement studies of complex samples, and studies of dilute phases.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics
Authors: Wejdemann, C. (Intern), Poulsen, H. F. (Intern)
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Scopus rating (2016): CiteScore 2.51 SJR 1.221 SNIP 1.211
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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
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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
Multiscale 3D characterization with dark-field x-ray microscopy

Dark-field x-ray microscopy is a new way to three-dimensionally map lattice strain and orientation in crystalline matter. It is analogous to dark-field electron microscopy in that an objective lens magnifies diffracting features of the sample; however, the use of high-energy synchrotron x-rays means that these features can be large, deeply embedded, and fully mapped in seconds to minutes. Simple reconfiguration of the x-ray objective lens allows intuitive zooming between different scales down to a spatial and angular resolution of 100 nm and 0.001 degrees, respectively. Three applications of the technique are presented-mapping the evolution of subgrains during the processing of plastically deformed aluminum, mapping domains and strain fields in ferroelectric crystals, and the three-dimensional mapping of strain fields around individual dislocations. This ability to directly characterize complex, multiscale phenomena in situ is a key step toward formulating and validating multiscale models that account for the entire heterogeneity of materials.
Nanodiamonds carrying silicon-vacancy quantum emitters with almost lifetime-limited linewidths

Colour centres in nanodiamonds are an important resource for applications in quantum sensing, biological imaging, and quantum optics. Here we report unprecedented narrow optical transitions for individual colour centres in nanodiamonds smaller than 200 nm. This demonstration has been achieved using the negatively charged silicon vacancy centre, which has recently received considerable attention due to its superb optical properties in bulk diamond. We have measured an ensemble of silicon-vacancy centres across numerous nanodiamonds to have an inhomogeneous distribution of 1.05 nm at 5 K. Individual spectral lines as narrower than 360 MHz were measured in photoluminescence excitation, and correcting for apparent spectral diffusion yielded an homogeneous linewidth of about 200 MHz which is close to the lifetime limit. These results indicate the high crystalline quality achieved in these nanodiamond samples, and advance the applicability of nanodiamond-hosted colour centres for quantum optics applications.
Solar energy is by far the most abundant renewable energy source available, but the levelized cost of solar energy is still not competitive with that of fossil fuels. Therefore there is a need to improve the power conversion efficiency of solar cells without adding to the production cost.

The main objective of this PhD thesis is to develop nanostructured silicon (Si) solar cells with higher power conversion efficiency using only scalable and cost-efficient production methods. The nanostructures, known as 'black silicon', are fabricated by single-step, maskless reactive ion etching and used as front texturing of different Si solar cells. Theoretically the nanostructure topology may be described as a graded refractive index in a mean-field approximation between air and Si. The optical properties of the developed black Si were simulated and experimentally measured. Total AM1.5G-weighted average reflectance well below 1% was measured for different crystalline grades of Si. Furthermore, the reflectance of RIE-textured Si remains below that of KOH-textured Si at all incident angles below 70°. RIE- and conventionally textured, screen-printed Si solar cells were fabricated on 156x156 mm² CZ Si wafers and characterized for comparison. Power
conversion efficiency of 16.5% was obtained for this batch of RIE-textured Si solar cells. The efficiency of the KOH-textured reference cell was 17.8%. Quantum Efficiency measurements and carrier loss analysis show that the lower efficiency of the RIE-textured cells is primarily due to increased emitter and surface recombination. The large-area screen-printed solar cells were furthermore characterized at varying incident angles. The angle-dependent analysis shows that RIE-textured cells have a higher normalized power output averaged over the range of incident angles between 0 and 90. This result indicates the potential of improved cell performance and higher output power at diffuse light conditions and during daily and yearly operation. A second batch of RIE-textured solar cells with laser-doped selective emitters (LDSE) was fabricated. A power conversion efficiency of 18.1% and a fill factor of 80.1% were obtained by laser doping and subsequent Ni/Cu plating in combination with RIE-texturing. This result shows the potential of improved efficiency of RIE-textured compared to conventionally textured cells, especially when laser doping on black Si is combined with improved surface passivation schemes such as atomic layer deposition (ALD) of Al₂O₃, ALD Al₂O₃ passivation on black Si yields surface recombination velocity (SRV) below 80 cm/s and implied open-circuit voltage (iVOC) of 680 mV. Surface recombination velocity of 20 cm/s and implied open-circuit voltage of 695 mV is obtained for black Si passivated by doped poly-Si and a tunnel oxide.

General information
State: Published
Organisations: Department of Micro- and Nanotechnology, Silicon Microtechnology, Experimental Surface and Nanomaterials Physics, Nanoprobes
Authors: Davidsen, R. S. (Intern), Hansen, O. (Intern), Boisen, A. (Intern), Schmidt, M. S. (Intern)
Number of pages: 236
Publication date: 2016

New catalysts for miniaturized methanol fuel cells
The methanol fuel cell is an interesting energy technology, capable of converting the chemical energy of methanol directly into electricity. The technology is specifically attractive for small mobile applications such as laptops, smartphones, tablets etc. since it offers almost instantaneously recharging by simply replacing the methanol liquid. The technology is currently being developed for hearing instruments in order to ease the handling of the device for users complaining about difficulties replacing the very small batteries in the hearing instrument. The technology has already been demonstrated by the Danish Technological Institute; however, for the technology to become more widely adapted, the power density of the fuel cell must be increased.

It is well known that a considerable part of the energy from the methanol is lost in the fuel cell during the conversion due to poor kinetics. The kinetics can however be improved by using a superior catalyst. Therefore, the aim of this thesis is to identify new catalyst material for methanol fuel cells. By analysing the performance of the standard catalysts (PtRu and Pt) currently being applied in methanol fuel cells as anode and cathode respectively, a benchmark is defined. This benchmark is used to compare catalysts for the different reactions taking place in a fuel cell such as hydrogen oxidation, methanol oxidation and oxygen reduction. In addition, different phenomena in the fuel cell such as CO poisoning of the hydrogen oxidation and methanol poisoning of the oxygen reduction are studied. Consequently, promising new candidates for replacing the standard catalyst are identified. One of these, Pt₅Gd, exhibits improved oxygen reduction reaction activity even in the presence of methanol, thus making Pt₅Gd an interesting candidate to replace the Pt catalyst in the methanol fuel cell cathode.

Having identified a potential new catalyst material, a fabrication method is needed. Because the catalytic properties of the catalyst material is inherent in the surface of the catalyst, the surface to volume ratio for the material must be as high as possible, which usually can only be achieved by making the material as nanoparticles. However, the problem of Pt₅Gd and other Pt alloys with lanthanides or early transition metals is that these materials are very difficult to synthesise chemically, especially in the more technological relevant nanoparticulate form. Therefore, a second objective of this thesis has been to investigate different synthesis routes. The thesis is able to demonstrate for the first time, chemical synthesised carbon supported metallic Pt₅Gd, Pt₅Y and Pt₅Tb alloy nanoparticles. The synthesised nanoparticles are more active than Pt nanoparticles, but not as active as expected for these materials. Thus, the synthesis route is promising but needs further optimisation.

General information
State: Published
Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics
Authors: Pedersen, C. M. (Intern), Chorkendorff, I. (Intern), Stephens, I. (Intern)
Number of pages: 188
New Insights into the Origins of Sb-Induced Effects on Self-Catalyzed GaAsSb Nanowire Arrays

Tertiary semiconductor nanowire arrays enable scalable fabrication of nano-optoelectronic devices with tunable bandgap. However, the lack of insight into the effects of the incorporation of V_y element results in lack of control on the growth of ternary III-V_{1-y}V_y nanowires and hinders the development of high-performance nanowire devices based on such ternaries. Here, we report on the origins of Sb-induced effects affecting the morphology and crystal structure of self-catalyzed GaAsSb nanowire arrays. The nanowire growth by molecular beam epitaxy is changed both kinetically and thermodynamically by the introduction of Sb. An anomalous decrease of the axial growth rate with increased Sb_2 flux is found to be due to both the indirect kinetic influence via the Ga adatom diffusion induced catalyst geometry evolution and the direct composition modulation. From the fundamental growth analyses and the crystal phase evolution mechanism proposed in this Letter, the phase transition/stability in catalyst-assisted ternary III-V-V nanowire growth can be well explained. Wavelength tunability with good homogeneity of the optical emission from the self-catalyzed GaAsSb nanowire arrays with high crystal phase purity is demonstrated by only adjusting the Sb_2 flux.
Noise robustness of a combined phase retrieval and reconstruction method for phase-contrast tomography

Classical reconstruction methods for phase-contrast tomography consist of two stages: phase retrieval and tomographic reconstruction. A novel algebraic method combining the two was suggested by Kostenko et al. [Opt. Express 21, 12185 (2013) [CrossRef], and preliminary results demonstrated improved reconstruction compared with a given two-stage method. Using simulated free-space propagation experiments with a single sample-detector distance, we thoroughly compare the novel method with the two-stage method to address limitations of the preliminary results. We demonstrate that the novel method is substantially more robust toward noise; our simulations point to a possible reduction in counting times by an order of magnitude.
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 (SIO), 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.

General information

State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Center for Individual Nanoparticle Functionality, Department of Micro- and Nanotechnology, Silicon Microtechnology, Department of Energy Conversion and Storage, Imaging and Structural Analysis, Experimental Surface and Nanomaterials Physics, Paul Scherrer Institut
Number of pages: 9
Pages: 455-463
Publication date: 2016
Main Research Area: Technical/natural sciences
Numerical and experimental study of the redistribution of energetic and impurity ions by sawteeth in ASDEX Upgrade: Paper

In the non-linear phase of a sawtooth, the complete reconnection of field lines around the $q = 1$ flux surface often occurs resulting in a radial displacement of the plasma core. A complete time-dependent electromagnetic model of this type of reconnection has been developed and implemented in the EBdyna_go code. This contribution aims at studying the behaviour of ions, both impurity and fast particles, in the pattern of reconnecting field lines during sawtoothing plasma experiments in the ASDEX Upgrade tokamak by using the newly developed numerical framework. Simulations of full reconnection with tungsten impurity that include the centrifugal force are achieved and recover the soft x-ray measurements. Based on this full-reconnection description of the sawtooth, a simple tool dedicated to estimate the duration of the reconnection is introduced. This work then studies the redistribution of fast ions during several experimentally observed sawteeth. In some cases of sawteeth at ASDEX Upgrade, full reconnection is not always observed or expected so the code gives an upper estimate of the actual experimental redistribution. The results of detailed simulations of the crashes are compared with measurements from various diagnostics such as collective Thomson scattering and fast-ion D-alpha (FIDA) spectroscopy, including FIDA tomography. A convincing qualitative agreement is found in different parts of velocity space.
Numerical modeling of the transition from low to high confinement in magnetically confined plasma

The transition dynamics from low (L) to high (H) mode confinement in magnetically confined plasmas is investigated using a four-field drift fluid model—HESEL (Hot Edge-Sol-Electrostatic). The model includes profile evolution and is solved in a 2D domain at the out-board mid-plane of a tokamak including both open and closed field lines. The results reveal different types of L–H-like transitions in response to ramping up the input power by increasing the ion temperature in the edge region. For a fast rising input power we obtain an abrupt transition, and for a slow rising power we obtain a L–I–H transition with an intermediate I-phase displaying limit-cycle oscillations (LCO). The model recovers the power threshold for the L–H transition, the scaling of the threshold with the density and with the loss-rate in the SOL, indicating a decrease in power threshold when switching from single to double null configuration. The results hold promises for developing full predictive modeling of the L–H transition, which is an essential step in understanding and optimizing fusion devices.
General information
State: Published
Organisations: Department of Physics, Plasma Physics and Fusion Energy, CAS - Institute of Plasma Physics, Instituto de Plasmas e Fusão Nuclear, Technical University of Denmark
Number of pages: 1
Publication date: 2016
Main Research Area: Technical/natural sciences
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Observing Solvation Dynamics with Simultaneous Femtosecond X-ray Emission Spectroscopy and X-ray Scattering
In liquid phase chemistry dynamic solute solvent interactions often govern the path, ultimate outcome, and efficiency of chemical reactions. These steps involve many-body movements on subpicosecond time scales and thus ultrafast structural tools capable of capturing both intramolecular electronic and structural changes, and local solvent structural changes are desired. We have studied the intra- and intermolecular dynamics of a model chromophore, aqueous [Fe(bpy)3]2+, with complementary X-ray tools in a single experiment exploiting intense XFEL radiation as a probe. We monitored the ultrafast structural rearrangement of the solute with X-ray emission spectroscopy, thus establishing time zero for the ensuing X-ray diffuse scattering analysis. The simultaneously recorded X-ray diffuse scattering attorns reveal slower subpicosecond dynamics triggered by the intramolecular structural dynamics of the photoexcited solute. By simultaneous combination of both methods only, we can extract new information about the solvation dynamic processes unfolding during the first picosecond (ps). The measured bulk solvent density increase of 0.2% indicates a dramatic change of the solvation shell around each photoexcited solute, confirming previous ab initio molecular dynamics simulations. Structural changes in the aqueous solvent associated with density and temperature changes occur with similar to 1 ps time constants, characteristic for structural dynamics in water. This slower time scale of the solvent response allows us to directly observe the structure of the excited solute molecules well before the solvent contributions become dominant.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Department of Chemistry, European XFEL, Paul Scherrer Institut, SLAC National Accelerator Laboratory, Hungarian Academy of Sciences, Lund University, European Synchrotron Radiation Facility
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Main Research Area: Technical/natural sciences
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.
On the pH dependence of electrochemical proton transfer barriers
The pH dependence of rate of the hydrogen evolution/oxidation reaction HER/HOR is investigated. Based on thermodynamic considerations, a possible explanation to the low exchange current for hydrogen reactions in alkaline is put forward. We propose this effect to be a consequence of the change in configurational entropy of the proton as it approaches the surface. As a proton crosses the outer Helmholtz plane, it will lose a fraction of its entropy before it can interact with the electrode surface, which gives rise to an entropic barrier. The size of this barrier will depend on the electrostatic environment in the double layer region. The entropic barrier can be rate determining only when the surface catalysis is fast. Therefore the effect of pH is most pronounced on good catalysts and for fast reactions. This entropic barrier is also in a good agreement with the unusually low prefactor measured in experiments of good catalysts such as Pt. In such catalysts, the enthalpy barrier of 0.1-0.2. eV of the rate-determining step does not come from any of the surface reactions (Volmer, Tafel or Heyrovsky) but instead from the proton transfer into the outer Helmholtz layer.
Opportunities and challenges in the electrocatalysis of CO2 and CO reduction using bifunctional surfaces: A theoretical and experimental study of Au-Cd alloys

Electrolysis could enable the large-scale conversion of CO2 to fuels and small molecules. This perspective discusses the state-of-the-art understanding of CO2 and CO reduction electrocatalysis and provides an overview of the most promising approaches undertaken thus far. We set to explore “bifunctional” catalysts using Au-Cd based alloys inspired by theoretical modelling. Density functional theory calculations suggest more favourable thermodynamics for CO2 reduction to CO and methanol on mixed Au-Cd sites on Au3Cd relative to similar values on Au. We use various tools to test the bulk and surface alloys experimentally. We find that Au3Cd in neutral media exhibits lower CO evolution activity than Au, and Au-Cd alloys also show negligible activity for CO reduction in alkaline media. This indicates that the mixed Cd-Au sites predicted to be catalytically active are not present in the sample. The catalytic performance is most consistent with Au-terminated step surface on a bulk alloy, possibly formed through adsorbate-induced restructuring. We highlight that future bimetallic catalysts must consider potential-dependent surface restructuring effects caused by reaction intermediates.

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BFI (2015): BFI-level 2
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Web of Science (2015): Indexed yes
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Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.553 SNIP 2.091 CiteScore 6.42
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Optical and acoustic sensing using Fano-like resonances in dual phononic and photonic crystal plate

We perform a theoretical study based on the transmissions of optical and acoustic waves normally impinging to a periodic perforated silicon plate when the embedded medium is a liquid and show the existence of Fano-like resonances in both cases. The signature of the resonances appears as well-defined asymmetric peaks in the phononic and photonic transmission spectra. We show that the origin of the Fano-like resonances is different with respect to the nature of the wave. In photonic, the origin comes from guided modes in the photonic plate while in phononic we show that it comes from the excitation of standing waves confined inside the cavity coming from the deformation of the water/silicon edges of the cylindrical inclusion. We finally use these features for sensing and show ultra-sensitivity to the light and sound velocities for different concentrations of analytes.

General information
State: Published
Organisations: Department of Physics, Biophysics and Fluids, Université Mouloud Mammeri, Université Lille Nord de France, Universite du Maine, Otto-von-Guericke University Magdeburg
Optical Biosensors to Explore Biological Systems

The study of live biological systems requires the use of advanced techniques that provide high structural and chemical information and at the same time, avoid damage in the system and modification of the structural/chemical features. Techniques based on interaction with light have shown their capability to work in biosensor devices. For example, Raman spectroscopy can be non-invasive and can provide 1 μm of spatial resolution in 1 second of collection time, well suited for sensing. Moreover, it may give information at the single cell and even approaching the single molecule scale. Here we present the capability of different light based techniques for biosensing.

As the first example, surface enhanced Raman spectroscopy (SERS) is performed in onion using silver plasmonic nanostructures. Our studies detect different molecular compounds present in the plant based on their SERS signals. SERS imaging allows us to monitor the location of nanoparticles and to image chemical compounds within the target. Moreover, a pH-sensitive reporter molecule, pMBA attached to the silver nanoparticles, is used to infer pH values in the extracellular space of an onion layer.

As a second example, we explore how a membrane protein may be used as an efficient sensor in an organic environment via a biomimetic membrane model. The combination of both biomimetic membranes and protein membranes as a signal transduction medium has interesting applications in biology and medicine. It is crucial that the matrix where a protein is embedded is optimal in order to maintain the concentration gradient. Moreover, curvature and mechanical forces in the membrane may also affect the protein function. In this work, by inducing chemical and mechanical changes of the matrix we optimize the system via measuring variations of the gradient through the membrane.

General information
State: Published
Organisations: Department of Physics, Biophysics and Fluids, Department of Environmental Engineering, Water Technologies, Philips Biocell, University of Copenhagen
Authors: Palanco, M. E. (Intern), Mogensen, K. B. (Ekstern), Andersen, N. H. S. (Ekstern), Berg-Sørensen, K. (Intern), Hélix-Nielsen, C. (Intern), Kneipp, K. (Intern)
Pages: 638A-639A
Publication date: 2016
Main Research Area: Technical/natural sciences

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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 0.979 SJR 1.949 CiteScore 3.15
Optical characterization of directly deposited graphene on a dielectric substrate

By using scanning multiphoton microscopy we compare the nonlinear optical properties of the directly deposited and transferred to the dielectric substrate graphene. The direct deposition of graphene on oxidized silicon wafer was done by utilizing sacrificial copper catalyst film. We demonstrate that the directly deposited graphene and bi-layered transferred graphene produce comparable third harmonic signals and have almost the same damage thresholds. Therefore, we believe directly deposited graphene is suitable for the use of e.g. nanofabricated optical setups. (C) 2016 Optical Society of America
Optically pumped 1550nm wavelength tunable MEMS VCSEL
The paper presents the design and fabrication of an optically pumped 1550nm tunable MEMS VCSEL with an enclosed MEMS. The MEMS is defined in SOI and the active material, an InP wafer with quantum wells are bonded to the SOI and the last mirror is made from the deposition of dielectric materials. The design brings flexibility to fabricate MEMS VCSELS over a wider range of wavelengths. The paper discusses results from the simulations and bonding results from fabrication. The device will push the boundaries for wavelength sweep speed and bandwidth.
Optical sensors and their applications for probing biological systems

There is a great interest in exploring and developing new optical sensitive methodologies for probing complex biological systems. In this project we developed non-invasive and sensitive biosensor strategies for studying physiologically relevant chemical and physical properties of plant and mammalian cells. First, we performed Surface Enhanced Raman Spectroscopy (SERS) studies on intact plant materials via using silver plasmonic nanostructures. Our studies showed strong Raman signals which resemble to the presence of typical constituents such as carbohydrates, proteins and lipids of different parts of the fresh tissues. The location of the nanoparticles inside some of the tissues was examined via SERS images, collected from Raman signatures of the constituents of the tissues as well as from Raman signatures of a specific pH-sensitive reporter molecule attached to the nanoparticles. The reporter molecule provided pH values of the extracellular space of the in-situ plant material.

The performance of SERS in intact plant tissues included the exploration of different strategies for synthesizing and delivering plasmonic nanostructures into plant tissues via green synthesis of silver nanoparticles with specific plants such as onions and fruit extracts. The formation of spherical and sharp-edged shape silver nanoparticles of around 10 to 300 nm showed the possibility of controlling the morphology of synthesized silver nanoparticles as a function of the plant extract used. Alternatively, the delivery of nanoparticles into the extracellular space of an intact plant tissue was carried out by the incubation of silver salts into the sample. Our results showed the formation of plasmonic nanostructures located at the extracellular space of the sample. This work showed the capability of an intact biological sample to provide a SERS-template where silver nanoparticles can grow, thus providing a new insight into SERS-based sensors for chemically sensing in-situ plant constituents.

Optical manipulation techniques have been used to investigate mechanical properties of soft membrane cells, i.e. mammalian cells, proteins and their interactions within a specific cell environment. Curvature and mechanical forces in the membrane play an important role in the activity of the membrane-bound protein. The overall motivation of the second part of the PhD project was to explore the dependence between the membrane curvature and the activity of membrane proteins. We developed an optical trapping device using a micro-fluidic chip with embedded delivery of laser light. The fluidic system consisted of three inlets joining to form a main channel that led to a single outlet. Cell samples were injected in the central inlet whereas side-inlets were used for hydrodynamic focusing in a stable-laminar flow in the chip. In the middle of the main channel, two optical fibers were placed opposite to one another and perpendicular to the axis of the main channel. Thus when a cell passes through the two opposing optical lasers, it can be trapped and deformed via variations of the light intensity through the optical fibers. Of key importance was the ability to create stable laminar flows at low velocity fields. We therefore optimized the presented device to be able to trap a large number of cells and to exchange the local environment of a trapped cell. The project could provide new insights into the desired biosensor for future membrane-protein cell studies.

General information
State: Published
Organisations: Department of Physics, Biophysics and Fluids
Authors: Palanco, M. E. (Intern), Kneipp, K. (Intern), Berg-Sørensen, K. (Intern), Hélix-Nielsen, C. (Intern)
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Projects:
Optical sensors and their applications for probing biological systems
Publication: Research › Ph.D. thesis – Annual report year: 2016

Optical two-beam trap in a polymer microfluidic chip
An optical two-beam trap, composed from two counter propagating laser beams, is an interesting setup due to the ability of the system to trap, hold, and stretch soft biological objects like vesicles or single cells. Because of this functionality, the system was also named “the optical stretcher” by Jochen Guck, Josep Käs and co-workers some 15 years ago. In a favorable setup, the two opposing laser beams meet with equal intensities in the middle of a fluidic channel in which cells may flow past, be trapped, stretched, and allowed to move on, giving the promise of a high throughput device. Yet, single beam optical traps, aka optical tweezers, by far outnumber the existing optical stretchers in research labs throughout the world. The ability to easily construct an optical stretcher setup in a low-cost material would possibly imply more frequent use of the optical stretching technique. Here, we will outline the design, the production procedures, and results obtained in a fiber-based experimental setup built within an injection molded microfluidic polymer chip. The microfluidic chip is constructed with a three layer technology in which we ensure both horizontal and vertical focusing of the cells we wish to
trap, thereby preventing too many cells to flow below the line of focus of the two counter propagating laser beams that are positioned perpendicular to the direction of flow of the cells. Results will be compared to that from other designs from previous work in the group.

**General information**
State: Published
Organisations: Department of Physics, Biophysics and Fluids, Department of Micro- and Nanotechnology, Optofluidics, Nanoprobes, NIL Technology ApS
Authors: Palanco, M. E. (Intern), Catak, D. (Intern), Marie, R. (Intern), Matteucci, M. (Intern), Bilenberg, B. (Ekstern), Kristensen, A. (Intern), Berg-Sørensen, K. (Intern)
Number of pages: 10
Publication date: 2016

**Host publication information**
Title of host publication: Proceedings of SPIE 9922, Optical Trapping and Optical Micromanipulation XIII
Volume: 9922
Publisher: SPIE - International Society for Optical Engineering

**Optical two-beam traps in microfluidic systems**
An attractive solution for optical trapping and stretching by means of two counterpropagating laser beams is to embed waveguides or optical fibers in a microfluidic system. The microfluidic system can be constructed in different materials, ranging from soft polymers that may easily be cast in a rapid prototyping manner, to hard polymers that could even be produced by injection molding, or to silica in which waveguides may either be written directly, or with grooves for optical fibers. Here, we review different solutions to the system and also show results obtained in a polymer chip with DUV written waveguides and in an injection molded polymer chip with grooves for optical fibers. (C) 2016 The Japan Society of Applied Physics.

**General information**
State: Published
Organisations: Department of Physics, Biophysics and Fluids
Authors: Berg-Sørensen, K. (Intern)
Number of pages: 4
Publication date: 2016
Main Research Area: Technical/natural sciences

**Publication information**
Volume: 55
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Article number: 08RA01
ISSN (Print): 0021-4922
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Web of Science (2018): Indexed yes
Scopus rating (2017): CiteScore 1.13 SJR 0.497 SNIP 0.668
Web of Science (2017): Indexed Yes
Scopus rating (2016): CiteScore 0.67 SJR 0.497 SNIP 0.768
Web of Science (2016): Indexed yes
Scopus rating (2015): SJR 0.426 SNIP 0.682 CiteScore 0.58
Scopus rating (2014): SJR 0.209 SNIP 0.189 CiteScore 0.73
Oscillating nonlinear acoustic shock waves

We investigate oscillating shock waves in a tube using a higher order weakly nonlinear acoustic model. The model includes thermoviscous effects and is non isentropic. The oscillating shock waves are generated at one end of the tube by a sinusoidal driver. Numerical simulations show that at resonance a stationary state arise consisting of multiple oscillating shock waves. Off resonance driving leads to a nearly linear oscillating ground state but superimposed by bursts of a fast oscillating shock wave. Based on a travelling wave ansatz for the fluid velocity potential with an added 2nd order polynomial in the space and time variables, we find analytical approximations to the observed single shock waves in an infinitely long tube. Using perturbation theory for the driven acoustic system approximative analytical solutions for the off resonant case are determined.

General information
State: Published
Organisations: Department of Physics, Department of Applied Mathematics and Computer Science, Dynamical Systems, Bogolyubov Institute for Theoretical Physics, GreenHydrogen.dk
Authors: Gaididei, Y. (Ekstern), Rasmussen, A. R. (Ekstern), Christiansen, P. L. (Intern), Sørensen, M. P. (Intern)
Number of pages: 15
Pages: 367-381
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Evolution Equations and Control Theory (Online)
Volume: 5
Issue number: 3
ISSN (Print): 2163-2480
Ratings:
Web of Science (2018): Indexed yes
Scopus rating (2017): SNIP 0.909 SJR 0.711 CiteScore 0.95
Web of Science (2017): Indexed Yes
Scopus rating (2016): SJR 0.999 SNIP 0.975 CiteScore 0.77
Parsing polarization squeezing into Fock layers

We investigate polarization squeezing in squeezed coherent states with varying coherent amplitudes. In contrast to the traditional characterization based on the full Stokes parameters, we experimentally determine the Stokes vector of each excitation subspace separately. Only for states with a fixed photon number do the methods coincide; when the photon number is indefinite, we parse the state in Fock layers, finding that substantially higher squeezing can be observed in some of the single layers. By capitalizing on the properties of the Husimi Q function, we map this notion onto the Poincare space, providing a full account of the measured squeezing.
General particle models with symmetric and asymmetric repulsion are studied and investigated for finite-range and exponential interaction in an annulus. In the symmetric case transitions from one- to multi-lane behavior including multistability are observed for varying particle density and for a varying curvature with fixed density. Hence, the system cannot be approximated by a periodic channel. In the asymmetric case, which is important in pedestrian dynamics, we reveal an inhomogeneous new phase, a traveling wave reminiscent of peristaltic motion.

**Pattern formation in annular systems of repulsive particles**

General particle models with symmetric and asymmetric repulsion are studied and investigated for finite-range and exponential interaction in an annulus. In the symmetric case transitions from one- to multi-lane behavior including multistability are observed for varying particle density and for a varying curvature with fixed density. Hence, the system cannot be approximated by a periodic channel. In the asymmetric case, which is important in pedestrian dynamics, we reveal an inhomogeneous new phase, a traveling wave reminiscent of peristaltic motion.

**General information**

State: Published

Organisations: Department of Applied Mathematics and Computer Science, Dynamical Systems, Department of Physics, Bogolyubov Institute for Theoretical Physics

Authors: Marschler, C. (Intern), Starke, J. (Intern), Sørensen, M. P. (Intern), Gaididei, Y. B. (Ekstern), Christiansen, P. L. (Intern)

Pages: 166-170

Publication date: 2016

Main Research Area: Technical/natural sciences

**Publication information**

Journal: Physics Letters A

Volume: 380

Issue number: 1-2

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Ratings:

BFI (2018): BFI-level 1

Web of Science (2018): Indexed yes

BFI (2017): BFI-level 1

Scopus rating (2017): SNIP 1.002 SJR 0.595 CiteScore 1.86
Performance Limits of Photoelectrochemical CO₂ Reduction Based on Known Electrocatalysts and the Case for Two-Electron Reduction Products

Solar-driven reduction of CO₂ to solar fuels as an alternative to H₂ via water splitting is an intriguing proposition. We model the solar-to-fuel (STF) efficiencies using realistic parameters based on recently reported CO₂ reduction catalysts with a high-performance tandem photoabsorber structure. CO and formate, which are both two-electron reduction products, offer STF efficiencies (20.0% and 18.8%) competitively close to that of solar H₂ (21.8%) despite markedly worse reduction catalysis. The slightly lower efficiency toward carbon products is mainly due to electrolyte resistance, not overpotential. Using a cell design where electrolyte resistance is minimized makes formate the preferred product from an efficiency standpoint (reaching 22.7% STF efficiency). On the other hand, going beyond a two-electron reduction reaction, the more highly reduced products seem unviable with presently available electrocatalysts due to excessive overpotentials and poor selectivity. This work considers breaking up the multielectron reduction pathway into individually optimized, separate two-electron steps as a way forward.

General information
State: Published
Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics
Authors: Vesborg, P. C. K. (Intern), Seger, B. (Intern)
Number of pages: 7
Pages: 8844-8850
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Chemistry of Materials
Volume: 28
Issue number: 24
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
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
Phase measurements exhibiting super sensitivity and super resolution features
By using an optical squeezed state and a post-processed homodyne detection scheme we show that phase measurements can overcome Rayleigh's resolution criterion and beat the quantum shot noise limit simultaneously.

General information
State: Published
Organisations: Department of Physics, Quantum Physics and Information Technology, Palacky University
Authors: Schäfermeier, C. (Intern), Jezek, M. (Ekstern), Gehring, T. (Intern), Andersen, U. L. (Intern)
Number of pages: 2
Pages: 1-2
Publication date: 2016

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Title of host publication: 2016 Conference on Lasers and Electro-optics
Publisher: I E E E
ISBN (Electronic): 9781943580118
Main Research Area: Technical/natural sciences
Conference: Conference on Lasers and Electro-Optics 2016, San Jose, California, United States, 05/06/2016 - 05/06/2016
Source: Findit
Source-ID: 2349999439
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2016

Phase Transition of MoS₂ Bilayer Structures
In the present study, using density functional calculations we have investigated a possible mechanism for the structural phase transition of the semiconducting bilayer 2H-MoS₂ via lithiation. The results indicate that the addition of lithium to the bilayer 2H-MoS₂ transforms the bilayer to a heterostructure of the 2H and 1T structures instead of a complete conversion to the 1T bilayer structure. Therefore, we propose that the desired synthesis of the 1T-MoS₂ from the bulk 2H-MoS₂ takes place through the hybrid 2H-1T structure. Our finding gives physical insight into the experimentally described microscopic mechanism of the phase transition in MoS₂ and enriches the atomic scale understanding of the interaction of MoS₂ with the alkali ions and other transition metal dichalcogenides manifesting a similar phase transition.
**pH in Grand Canonical Statistics of an Electrochemical Interface**

We present an atomic-scale model of the electrochemical interface, which unfolds the effects of pH and electrode potential using a generalized computational hydrogen electrode. The liquid structure of the solvent is included with the use of ab initio molecular dynamics to sample thousands of microstates with varying numbers of protons and electrons. The grand canonical probability weight function at constant pH and electrode potential is calculated a posteriori. The only inputs to the model are the fundamental assumptions of an equilibrated solvent, charge neutrality of the interface, and the dimensions of the system. The structures are unbiased outputs, and several atomic-scale quantities are calculated for our model system, water/Au(111), as weighted averages. We present the potentials of zero charge, Gibbs isotherms, and differential capacities as a function of pH. The potential of maximum entropy is also calculated, which to our knowledge has not previously been done with any first-principles method. The model predicts a non-Nernstian pH behavior for the potential of maximum entropy.

**General information**
- State: Published
- Organisations: Department of Physics, Theoretical Atomic-scale Physics, University of Copenhagen
- Authors: Hansen, M. H. (Intern), Rossmeisl, J. (Ekstern)
- Number of pages: 9
- Pages: 29135-29143
- Publication date: 2016
- Main Research Area: Technical/natural sciences

**Publication information**
- Volume: 120
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- ISSN (Print): 1089-5639
- Ratings:
  - BFI (2018): BFI-level 1
  - Web of Science (2018): Indexed yes
  - BFI (2017): BFI-level 1
  - Scopus rating (2017): CiteScore 2.75
  - Web of Science (2017): Indexed yes
  - BFI (2016): BFI-level 1
  - Scopus rating (2016): CiteScore 2.64
  - Web of Science (2016): Indexed yes
  - BFI (2015): BFI-level 1
  - Scopus rating (2015): CiteScore 2.78
  - Web of Science (2015): Indexed yes
  - BFI (2014): BFI-level 1
  - Scopus rating (2014): CiteScore 2.65
  - Web of Science (2014): Indexed yes
  - BFI (2013): BFI-level 1
  - Scopus rating (2013): CiteScore 2.84
  - ISI indexed (2013): ISI indexed yes
  - Web of Science (2013): Indexed yes
  - BFI (2012): BFI-level 1
  - Scopus rating (2012): CiteScore 2.78
  - ISI indexed (2012): ISI indexed yes
  - Web of Science (2012): Indexed yes
Pollen, water, and wind: Chaotic mixing in a puddle of water

This paper talks about how pine pollen grains dispersed in an approximately 1 m wide and 1 cm deep water puddle. The pollen has mixed due to wind blowing across the liquid surface, revealing a strikingly complex flow pattern. The flows revealed by nature’s tracer particles may influence circulation and nutrient distribution in puddles and small ponds. The flow patterns are generated by wind blowing across the puddle surface. This causes a shear stress at the atmospheric interface, which drives a flow in the liquid below. Chaotic mixing can occur if the wind direction changes over time. A fluid patch is repeatedly stretched and folded into itself, resulting in a drastic reduction of the length over which molecules have to diffuse. Pollen from pine trees was unusually abundant in 2012 when the photograph was taken, due to a largely dry spring which brought more than usual. Pine pollen is winged, and typically measures ~50 μm in diameter. Pollen is transferred from a pollen cone to the ovule by wind or insects, and produces male sperm cells
Precipitation pathways for ferrihydrite formation in acidic solutions
Iron oxides and oxyhydroxides form via Fe$^{3+}$ hydrolysis and polymerization in many aqueous environments, but the pathway from Fe$^{3+}$ monomers to oligomers and then to solid phase nuclei is unknown. In this work, using combined X-ray, UV-vis, and Mossbauer spectroscopic approaches, we were able to identify and quantify the long-time sought ferric speciation over time during ferric oxyhydroxide formation in partially-neutralized ferric nitrate solutions ([Fe$^{3+}$] = 0.2 M, 1.8 <pH <3). Results demonstrate that Fe exists mainly as Fe(H$_2$O)$_6^{3+}$, mu-oxo aquo dimers and ferrihydrite, and that with time, the mu-oxo dimer decreases while the other two species increase in their concentrations. No larger Fe oligomers were detected. Given that the structure of the mu-oxo dimer is incompatible with those of all Fe oxides and oxyhydroxides, our results suggest that reconfiguration of the mu-oxo dimer structure occurs prior to further condensation leading up to the nucleation of ferrihydrite. The structural reconfiguration is likely the rate-limiting step involved in the nucleation process.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, University of Wyoming, University of Delaware, University of California at Berkeley, Lawrence Berkeley National Laboratory
Number of pages: 18
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Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Geochimica Et Cosmochimica Acta
Volume: 172
ISSN (Print): 0016-7037
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 4.85
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.42
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 4.55
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 4.48
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 4.48
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 3.93
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 4.01
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
Probing the local, electronic and magnetic structure of matter under extreme conditions of temperature and pressure

In this paper we present recent achievements in the field of investigation of the local, electronic and magnetic structure of the matter under extreme conditions of pressure and temperature. These results were obtained thanks to the coupling of a compact laser heating system to the energy-dispersive XAS technique available on the ID24 beamline at the ESRF synchrotron. The examples chosen concern the melting and the liquid structure of 3d metals and alloys under high pressures (HPs) and the observation of temperature-induced spin crossover in FeCO$_3$ at HP.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, European Synchrotron Radiation Facility, Sorbonne Universités, Ehime University
Authors: Torchio, R. (Ekstern), Boccato, S. (Ekstern), Cerantola, V. (Ekstern), Morard, G. (Ekstern), Irifune, T. (Ekstern), Kantor, I. (Intern)
Number of pages: 10
Pages: 293-302
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: High Pressure Research
Volume: 36
Issue number: 3
ISSN (Print): 0895-7959
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 0.982 SJR 0.69 CiteScore 1.62
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.12 SJR 0.388 SNIP 0.69
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.458 SNIP 0.804 CiteScore 1.08
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.503 SNIP 0.673 CiteScore 0.99
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.447 SNIP 0.66 CiteScore 1.03
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.471 SNIP 0.502 CiteScore 0.82
Probing the nanoscale structure of the catalytically active overlayer on Pt alloys with rare earths

PtxY and PtxGd exhibit exceptionally high activity for oxygen reduction, both in the polycrystalline form and the nanoparticulate form. In order to understand the origin of the enhanced activity of these alloys, we have investigated thin films of these alloys on bulk Pt(111) crystals, i.e. Y/Pt(111) and Gd/Pt(111). These surfaces exhibit a 4-fold improvement over Pt(111). We observe the formation of a thick Pt overlayer after the electrochemical measurements, both on Y/Pt(111) and Gd/Pt(111). Using surface sensitive X-ray diffraction we revealed that crystalline closely packed Pt overlayers were formed. The diffraction experiments showed that the strain and crystallinity of the overlayers are strongly dependent on the electrochemical treatment, and in general show lateral compression.
Protection of Si photocathode using TiO₂ deposited by high power impulse magnetron sputtering for H₂ evolution in alkaline media

Si is an excellent absorber material for use in photoelectrochemical (PEC) hydrogen production. Only a few studies have been done using Si in alkaline electrolyte for hydrogen evolution due to its poor chemical stability in high pH electrolyte, indicating that a chemically stable protection layer is essential. Here we investigate thin TiO₂ films deposited by high power impulse magnetron sputtering (HiPIMS) as a protection layer for a p-type silicon photocathode for photoelectrochemical H₂ evolution in a high pH electrolyte. The X-ray reflectometry analysis reveals that the HiPIMS process provides improved film density for TiO₂ films (4.15 g/cm³), and consequently results in a significantly less corroded Si surface. The Si photocathode protected by the HiPIMS grown TiO₂ film along with Pt as co-catalyst produced a photocurrent onset potential of ~0.5 V vs. RHE in 1 M KOH and showed a 4% decay over 24 h in KOH. In contrast, the sample with the TiO₂ deposited using conventional DC sputtering technique of similar thickness shows 20% loss in photocurrent for the same time interval. Considering the fact that the experiments were carried out not in the cleanroom, much less corrosion loss can be obtained if done in dust-free condition. Hence, these results suggest the HiPIMS technique as an improved approach for the protection of photoelectrodes, which are unstable in alkaline solution.

General information
State: Published
Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics, Department of Micro- and Nanotechnology, Silicon Microtechnology, University of Iceland
Authors: Bae, D. (Intern), Shayestehaminzadeh, S. (Ekstern), Thorsteinsson, E. B. (Ekstern), Pedersen, T. (Intern), Hansen, O. (Intern), Seger, B. (Intern), Vesborg, P. C. K. (Intern), Ólafsson, S. (Ekstern), Chorkendorff, I. (Intern)
Pages: 758-765
Publication date: 2016
Main Research Area: Technical/natural sciences

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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): SNIP 1.532 SJR 1.459 CiteScore 4.83
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.97 SJR 1.599 SNIP 1.71
Pt-based Thin Films as Efficient and Stable Catalysts for Oxygen Electroreduction

This thesis presents the fabrication and characterization of Pt-based thin film catalysts for Oxygen Reduction Reaction (ORR). Gadolinium and Yttrium have been used as alloying materials, in preparation for the replacement of the traditional but economically disadvantageous pure Pt catalysts at the cathode of Polymer Electrolyte Membrane Fuel Cells (PEMFCs).

Herein the fabrication method, which consists of co-sputtering of thin films, is presented in detail, explaining the challenges
one must face in order to fabricate oxygen-free Pt-lanthanides and Pt-early transition metals alloys, and the proposed solutions. The characterization of the catalysts focused mainly on the electrochemical testing using a Rotating Ring Disk Electrode (RRDE) setup, and includes X-ray Diffraction (XRD), X-ray Photoemission Spectroscopy (XPS), Angle-Resolved X-ray Photoelectron Spectroscopy (AR-XPS), Scanning Electron Microscopy (SEM), Energy Dispersive X-ray spectroscopy (EDX) and Inductively Coupled Plasma Mass Spectroscopy (ICP-MS).

The investigated films included pure Pt sputtered thin films, as well as PtGd and PtY thin film alloys of different compositions and thicknesses, with the aim of a model study to pursue more active and stable ORR catalysts. While the Pt and PtGd films were deposited at DTU Physics, the PtY alloys were fabricated at Chalmers University, which has been collaborating in the NACORR project.

When tested electrochemically, 50 nm thick PtGd thin film catalysts exhibited a 4.5-fold enhancement in activity at 0.9 V vs. Reversible Hydrogen electrode (RHE) compared with polycrystalline Pt. This value increases to a 7-fold enhancement for 30 nm thick PtY films. Moreover, pure Pt thin films showed an activity which was roughly double the one recorded for polycrystalline Pt, and this could be due to the different kind of surfaces generated by sputtering. Both the PtGd and PtY films maintain over 80 % of the initial ORR activity when cycled 10000 times between 0.6 and 1.0 V vs. RHE in 0.1 M HClO4, and that is an indicator of the good stability of these catalysts. Investigation of the films through XRD showed that a metallic alloy structure is formed, matching the structure of polycrystalline samples. XPS and EDX analyses confirmed the composition of the alloys, proving good control of the co-deposition rates of the sputter chamber. With this techniques, it was possible to observe the formation of a thick, strained Pt overlayer, which is probably responsible for the activity enhancement.

A study of the thickness of PtY alloys revealed that the thin film formation during sputtering happened by island growth, and showed that smooth films were obtained when the thickness was equal or above 27 nm. A brief study was conducted at Stanford University, in collaboration with the Jaramillo group and SLAC, on Pt and PtGd films deposited via evaporation. The results underlined the importance of an oxygen-free environment when dealing with Pt-lanthanides thin film fabrication.
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

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

QMC approach based on the Bogoliubov independent quark model of the nucleon

General information
State: Published
Organisations: Department of Physics, University of California, Los Angeles, Utkal University, Universidade de Coimbra
Authors: Bohr, H. (Intern), Moszkowski, S. A. (Ekstern), Panda, P. K. (Ekstern), Providência, C. (Ekstern), da Providência, J. (Ekstern)
Number of pages: 13
Publication date: 2016
Main Research Area: Technical/natural sciences

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Volume: 25
Issue number: 2
Article number: 1650007
ISSN (Print): 0218-3013
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 0.816 SJR 0.687 CiteScore 1.2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.18 SJR 0.789 SNIP 0.781
Web of Science (2016): Indexed yes
Quantifying the onset of recrystallization in deformed metals using x-rays

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics
Authors: Ahl, S. R. (Intern), Simons, H. (Intern), Poulsen, H. F. (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-4
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2016

Quantifying the promotion of Cu catalysts by ZnO for methanol synthesis
Promoter elements enhance the activity and selectivity of heterogeneous catalysts. Here, we show how methanol synthesis from synthesis gas over copper (Cu) nanoparticles is boosted by zinc oxide (ZnO) nanoparticles. By combining surface area titration, electron microscopy, activity measurement, density functional theory calculations, and modeling, we
show that the promotion is related to Zn atoms migrating in the Cu surface. The Zn coverage is quantitatively described as a function of the methanol synthesis conditions and of the size-dependent thermodynamic activities of the Cu and ZnO nanoparticles. Moreover, experimental data reveal a strong interdependency of the methanol synthesis activity and the Zn coverage. These results demonstrate the size-dependent activities of nanoparticles as a general means to design synergetic functionality in binary nanoparticle systems.

**General information**

State: Published
Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics, Haldor Topsoe AS
Authors: Kuld, S. (Ekstern), Thorhauge, M. (Ekstern), Falsig, H. (Ekstern), Elkjær, C. F. (Intern), Helveg, S. (Ekstern), Chorkendorff, I. (Intern), Sehested, J. (Ekstern)
Number of pages: 6
Pages: 969-974
Publication date: 2016
Main Research Area: Technical/natural sciences

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Journal: Science (New York, N.Y.)
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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
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Web of Science (2012): Indexed yes
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Scopus rating (2011): SJR 14.238 SNIP 8.277 CiteScore 11.97
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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
Quantum enhanced optical sensing

The work in this thesis is embedded in the framework of quantum metrology and explores quantum effects in solid state emitters and optical sensing. Specifically, the thesis comprises studies on silicon vacancy centres in nanodiamonds, phase measurements and cavity optomechanics utilising optical squeezed states, and a theoretical study on quantum amplifiers.

Due to its similarity to single atoms, colour centres in diamond are ideal objects for exploring and exploiting quantum effects, because they are comparably easy to produce, probe and maintain. While nitrogen vacancy centres are the most renowned colour centres, we studied the silicon vacancy (SiV−) centre. In bulk diamond it features strong zero-phonon-line emission and, at cryogenic temperatures, a linewidth of hundreds of MHz, but it displays a weak spin coherence in the order of ns. To suppress the relaxation process which limits the coherence time, we utilised SiV− centres in nanodiamond. By means of confocal microscopy and resonant excitation at cryogenic temperatures, we measured linewidths in recently developed nanodiamond which were an order of magnitude smaller compared to previous studies on SiV− nanodiamonds. Furthermore, we identified spectral diffusion as the main hindrance in extending spin coherence times. Overcoming this issue will provide a promising candidate as an emitter for quantum information. Next, the question of how squeezed states of light can improve optical sensing was addressed. For this purpose, a squeezed light source was designed and built from scratch, which achieved a noise suppression of −8 dB at an optical pump power of 40mW. The generated squeezed light was first used to demonstrate how Gaussian states and detection can beat the shot noise limit and Rayleigh criterion in phase measurements simultaneously. Compared to quantum phase measurements based on single photon states, this approach is inherently deterministic. In addition, the applied homodyne detection enables close-to-unity detection efficiencies and thereby outperforms single photon state strategies which rely on comparably inefficient or demanding detection techniques.

A second experiment combined squeezed light and feedback control to cool an optomechanical system. This proof-of-principle study is the first reported squeezing enhanced optomechanical cooling experiment. Despite losses of more than 50% (a resulting noise suppression of −2 dB), the mechanical resonator was cooled from room temperature to 130K. This represents a 12% improvement compared to the use of a coherent state protocol. Finally, we theoretically investigated the fundamental properties of quantum amplifiers. Such devices can be used in information and sensing technology to amplify signals to overcome e.g. technical detection limitations. Amplified communication channels were characterised by applying the measure of mutual information I, as it offers strict bounds on the maximum achievable performance, which enabled a fair comparison between different applications scenarios. As a result, we identified two peculiar configurations: A configuration where amplification does not affect I, and a configuration where quantum correlations do not always lead to an enhanced I.

General information
State: Published
Organisations: Department of Physics, Quantum Physics and Information Technology
Authors: Schäfermeier, C. (Intern), Andersen, U. L. (Intern), Huck, A. (Intern)
Number of pages: 200
Quantum Information Protocols with Gaussian States of Light

Quantum cryptography is widely regarded as the most mature field within the context of quantum information in the sense that its application and development has produced companies that base their products on genuine quantum mechanical principles. Examples include quantum random number generators and hardware for secure quantum key distribution. These technologies directly exploit quantum effects, and indeed this is where they offer advantages to classical products. This thesis deals with the development and implementation of quantum information protocols that utilize the rather inexpensive resource of Gaussian states. A quantum information protocol is essentially a sequence of state exchanges between some number of parties and a certain ordering of quantum mechanical unitary operators performed by these parties. An example of this is the famous BB84 protocol for secret key generation, where photons in different polarization states are sent from one party to the other and subsequently detected.

In particular we introduce the idea of measurement device independence for continuous variable states and we present a proof-of-principle implementation of this protocol. Measurement device independence with Gaussian states is a promising avenue for the development of practical quantum key distribution with a relay network structure in environments where the distances are relatively short and there is a high number of users, such as an urban environment.

In addition to this we consider various point-to-point configurations that utilize Gaussian states to achieve security. Notably, we also present a novel experiment demonstrating the feasibility of delegated quantum computing on encrypted data, where we show that we can reliably encrypt and decrypt input and output states when a server with quantum computing capabilities performs Gaussian operations.
Random-phase metasurfaces at optical wavelengths

Random-phase metasurfaces, in which the constituents scatter light with random phases, have the property that an incident plane wave will diffusely scatter, hereby leading to a complex far-field response that is most suitably described by statistical means. In this work, we present and exemplify the statistical description of the far-field response, particularly highlighting how the response for polarised and unpolarised light might be alike or different depending on the correlation of scattering phases for two orthogonal polarisations. By utilizing gap plasmon-based metasurfaces, consisting of an optically thick gold film overlaid by a subwavelength thin glass spacer and an array of gold nanobricks, we design and realize random-phase metasurfaces at a wavelength of 800 nm. Optical characterisation of the fabricated samples convincingly demonstrates the diffuse scattering of reflected light, with statistics obeying the theoretical predictions. We foresee the use of random-phase metasurfaces for camouflage applications and as high-quality reference structures in dark-field microscopy, while the control of the statistics for polarised and unpolarised light might find usage in security applications. Finally, by incorporating a certain correlation between scattering by neighbouring metasurface constituents new types of functionalities can be realised, such as a Lambertian reflector.
Relation between Hydrogen Evolution and Hydrodesulfurization Catalysis

A relation between hydrogen evolution and hydrodesulfurization catalysis was found by density functional theory calculations. The hydrogen evolution reaction and the hydrogenation reaction in hydrodesulfurization share hydrogen as a surface intermediate and, thus, have a common elementary step, which indicates that the same catalyst should perform well for both hydrogen evolution and hydrogenation. If that catalyst also fulfills additional criteria for breaking carbon–sulfur bonds and releasing hydrogen sulfide, it will be a good hydrodesulfurization catalyst. The hydrogen evolution reaction is normally performed at room temperature and standard pressure, whereas the hydrodesulfurization reaction is driven by high temperature and pressure. Owing to the very different operating conditions, the adsorption free energy of hydrogen differs between hydrodesulfurization and the hydrogen evolution reaction, which makes the connection between the two less obvious.
Reproducibility in density functional theory calculations of solids

The widespread popularity of density functional theory has given rise to an extensive range of dedicated codes for predicting molecular and crystalline properties. However, each code implements the formalism in a different way, raising questions about the reproducibility of such predictions. We report the results of a community-wide effort that compared 15 solid-state codes, using 40 different potentials or basis set types, to assess the quality of the Perdew-Burke-Ernzerhof equations of state for 71 elemental crystals. We conclude that predictions from recent codes and pseudopotentials agree very well, with pairwise differences that are comparable to those between different high-precision experiments. Older methods, however, have less precise agreement. Our benchmark provides a framework for users and developers to document the precision of new applications and methodological improvements.
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Scopus rating (2009): SJR 11.897 SNIP 7.056
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Scopus rating (2008): SJR 11.277 SNIP 6.075
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Scopus rating (2007): SJR 10.072 SNIP 6.017
Web of Science (2007): Indexed yes
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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
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Web of Science (2000): Indexed yes
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Revealing the Formation of Copper Nanoparticles from a Homogeneous Solid Precursor by Electron Microscopy
The understanding of processes leading to the formation of nanometer-sized particles is important for tailoring of their size, shape and location. The growth mechanisms and kinetics of nanoparticles from solid precursors are, however, often poorly described. Here we employ transmission electron microscopy (TEM) to examine the formation of copper nanoparticles on a silica support during the reduction by $\text{H}_2$ of homogeneous copper phyllosilicate platelets, as a prototype precursor for a coprecipitated catalyst. Specifically, time-lapsed TEM image series acquired of the material during the reduction process provide a direct visualization of the growth dynamics of an ensemble of individual
nanoparticles and enable a quantitative evaluation of the nucleation and growth of the nanoparticles. This quantitative information is compared with kinetic models and found to be best described by a nucleation-and-growth scenario involving autocatalytic reduction of the copper phyllosilicate followed by diffusion-limited or reaction-limited growth of the copper nanoparticles. The plate-like structure of the precursor restricted the diffusion of copper and the autocatalytic reduction limited the probability for secondary nucleation. The combination of a uniform size of precursor particles and the autocatalytic reduction thus offers means to synthesize nanoparticles with well-defined sizes in large amounts. In this way, in situ observations made by electron microscopy provide mechanistic and kinetic insights into the formation of supported nanoparticles, essential for the rational design of nanomaterials.

**General information**
State: Published
Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics, Haldor Topsoe AS, Utrecht University, University of Liège
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): SNIP 2.641 SJR 8.127 CiteScore 14.05
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 13.18 SJR 7.492 SNIP 2.596
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BFI (2015): BFI-level 2
Scopus rating (2015): SJR 6.775 SNIP 2.63 CiteScore 12.81
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 6.294 SNIP 2.587 CiteScore 11.92
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 5.993 SNIP 2.466 CiteScore 11.38
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 6.211 SNIP 2.38 CiteScore 10.37
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 5.478 SNIP 2.321 CiteScore 9.94
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 5.167 SNIP 2.138
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
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Reversible Polarization Rotation in Epitaxial Ferroelectric Bilayers
Polarization rotation engineering is a promising path to giant dielectric and electromechanical responses in ferroelectric materials and devices. This work demonstrates robust and reversible in- to out-of-plane polarization rotation in ultrathin (nanoscale) epitaxial (001) tetragonal PbZr_{0.3}Ti_{0.7}O_{3} (PZT-T)/rhombohedral PbZr_{0.55}Ti_{0.45}O_{3} (PZT-R) ferroelectric bilayers. An underlying 20 nm thick PZT-R layer reduces the symmetry in a 5 nm thick PZT-T layer by imposing an in-plane tensile strain while simultaneously decoupling the PZT-T layer from the substrate. This prevents clamping and facilitates large-scale polarization rotation switching (=60 μC cm\(^{-2}\)) and an effective \(d_{33}\) response 500% (=250 pm V\(^{-1}\)) larger than the PZT-R layer alone. Furthermore, this enhancement is stable for more than 10\(^7\) electrical switching cycles. These bilayers present a simple and highly controllable means to design and optimize rotational polar systems as an alternate to traditional composition-based approaches. The precise control of the subtle interface-driven interactions between the lattice and the external factors that control polarization opens a new door to enhanced—or completely new—functional properties.

General information
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Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, University of New South Wales, Pennsylvania State University
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Robust structural identification via polyhedral template matching
Successful scientific applications of large-scale molecular dynamics often rely on automated methods for identifying the local crystalline structure of condensed phases. Many existing methods for structural identification, such as common neighbour analysis, rely on interatomic distances (or thresholds thereof) to classify atomic structure. As a consequence they are sensitive to strain and thermal displacements, and preprocessing such as quenching or temporal averaging of the atomic positions is necessary to provide reliable identifications. We propose a new method, polyhedral template matching (PTM), which classifies structures according to the topology of the local atomic environment, without any ambiguity in the classification, and with greater reliability than e.g. common neighbour analysis in the presence of thermal fluctuations. We demonstrate that the method can reliably be used to identify structures even in simulations near the melting point, and that it can identify the most common ordered alloy structures as well. In addition, the method makes it easy to identify the local lattice orientation in polycrystalline samples, and to calculate the local strain tensor. An implementation is made available under a Free and Open Source Software license.

General information
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Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Experimental Surface and Nanomaterials Physics
Authors: Larsen, P. M. (Intern), Schmidt, S. (Intern), Schiøtz, J. (Intern)
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Scopus rating (2017): SNIP 0.93 SJR 0.821 CiteScore 1.8
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 1.82 SJR 1.076 SNIP 1.05
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BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.225 SNIP 1.057 CiteScore 1.73
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.305 SNIP 1.157 CiteScore 1.81
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Room temperature Up-conversion detection of a broadband Mid-IR source
The paper presents efficient up-conversion based room temperature detection of a broadband mid-infrared light source, ranging from 3.6 ~ 4.9 μm, exploiting nonlinear sum frequency generation in a periodically poled lithium-niobate crystal.
Sap flow and sugar transport in plants

Green plants are Earth's primary solar energy collectors. They harvest the energy of the Sun by converting light energy into chemical energy stored in the bonds of sugar molecules. A multitude of carefully orchestrated transport processes are needed to move water and minerals from the soil to sites of photosynthesis and to distribute energy-rich sugars throughout the plant body to support metabolism and growth. The long-distance transport happens in the plants' vascular system, where water and solutes are moved along the entire length of the plant. In this review, the current understanding of the mechanism and the quantitative description of these flows are discussed, connecting theory and experiments as far as possible. The article begins with an overview of low-Reynolds-number transport processes, followed by an introduction to the anatomy and physiology of vascular transport in the phloem and xylem. Next, sugar transport in the phloem is explored with attention given to experimental results as well as the fluid mechanics of osmotically driven flows. Then water transport in the xylem is discussed with a focus on embolism dynamics, conduit optimization, and couplings between water and sugar transport. Finally, remarks are given on some of the open questions of this research field. Green plants harvest the energy of the Sun in the leaves by converting light energy into chemical energy in the bonds of sugar molecules, using water from the soil and carbon dioxide from the air. This review provides an overview of the vascular anatomy of plants and the physical models that describe the long-distance transport of water and minerals from root to leaf, and, in particular, of sugars from the leaves to the entire body of the plant sustaining growth and communication throughout even the tallest tree.
We have studied the interaction of 8-hydroxyquinoline-5-sulfonate (8-HQS) with the metal ions Al(III) and Zn(II) in aqueous solution in the presence of tetraalkylammonium surfactants using UV/vis absorption, fluorescence, NMR spectroscopy and electrical conductivity measurements, complemented by DFT calculations and molecular dynamics (MD) simulations. Under appropriate conditions, complexes between 8-HQS and metal ions form rapidly, and have similar electronic, spectroscopic and photophysical properties to the corresponding metal quinolates, such as Alq3. These interact with the cationic surfactants, leading to marked increases in fluorescence intensity. However, significant differences are seen in the behavior of the two metal ions. With aluminum, a stable [Al(8-QS)3]3- anion is formed, and interacts, predominantly through electrostatic interactions, with the surfactant, without disrupting the metal ion coordination sphere. In contrast, with Zn(II), there is a competition between the metal ion and surfactants in the interaction with 8-HQS, although the [Zn(8-QS)2(H2O)2]2+ species is stable at appropriate pH and surfactant concentration. The studies are extended to systems with the conjugated polyelectrolyte (CPE) poly-(9,9-bis(6-N, N, N-trimethylammonium) hexyl)-fluorene-phenylene bromide (HTMA-PFP), which has a similar alkylammonium chain to the surfactants. Mixing metal salt, 8-HQS and HTMA-PFP in the presence of a nonionic surfactant leads to the formation of a metal complex/CPE supramolecular assembly between the conjugated polyelectrolyte and the metal/8-HQS complex, as demonstrated by electronic energy transfer. The potential of these systems in sensing, light harvesting, and electron injection/transport layers in organic semiconductor devices is discussed.
Shielding efficiency of metal hydrides and borohydrides in fusion reactors

Mass attenuation coefficients, mean free paths and exposure buildup factors have been used to characterize the shielding efficiency of metal hydrides and borohydrides, with high density of hydrogen. Gamma ray exposure buildup factors were computed using five-parameter geometric progression fitting at energies 0.015 MeV to 15 MeV, and for penetration depths up to 40 mean free paths. Fast-neutron shielding efficiency has been characterized by the effective neutron removal cross-section. It is shown that ZrH₂ and VH₂ are very good shielding materials for gamma rays and fast neutrons due to their suitable combination of low- and high-Z elements. The present work should be useful for the selection and design of blankets and shielding, and for dose evaluation for components in fusion reactors.

General information
State: Published
Organisations: Department of Physics, Karnatak University
Authors: Singh, V. P. (Ekstern), Badiger, N. M. (Ekstern), Gerward, L. (Intern)
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Web of Science (2016): Indexed yes
Scopus rating (2015): SJR 0.28 SNIP 0.38 CiteScore 0.42
Scopus rating (2014): SJR 0.331 SNIP 0.657 CiteScore 0.58
Scopus rating (2013): SJR 0.345 SNIP 0.935 CiteScore 1.07
Scopus rating (2012): SJR 0.335 SNIP 1.037 CiteScore 1.04
Scopus rating (2011): SJR 0.296 SNIP 1.223 CiteScore 1.02
Scopus rating (2010): SJR 0.349 SNIP 0.74
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Simple Screened Hydrogen Model of Excitons in Two-Dimensional Materials

We present a generalized hydrogen model for the binding energies (EB) and radii of excitons in two-dimensional (2D) materials that sheds light on the fundamental differences between excitons in two and three dimensions. In contrast to the well-known hydrogen model of three-dimensional (3D) excitons, the description of 2D excitons is complicated by the fact that the screening cannot be assumed to be local. We show that one can consistently define an effective 2D dielectric constant by averaging the screening over the extend of the exciton. For an ideal 2D semiconductor this leads to a simple expression for EB that only depends on the excitonic mass and the 2D polarizability α. The model is shown to produce accurate results for 51 transition metal dichalcogenides. Remarkably, over a wide range of polarizabilities the binding energy becomes independent of the mass and we obtain $E_{2DB} \approx 3/(4\pi\alpha)$, which explains the recently observed linear scaling of exciton binding energies with band gap. It is also shown that the model accurately reproduces the nonhydrogenic Rydberg series in WS2 and can account for screening from the environment.

General information
State: Published
Organisations: Center for Atomic-scale Materials Design, Department of Physics, Center for Nanostructured Graphene
Authors: Olsen, T. (Intern), Latini, S. (Intern), Rasmussen, F. A. (Intern), Thygesen, K. S. (Intern)
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Scopus rating (2016): CiteScore 6.33 SJR 4.196 SNIP 2.61
Web of Science (2016): Indexed yes
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BFI (2014): BFI-level 2
Scopus rating (2014): SJR 5.232 SNIP 2.71 CiteScore 6.62
Web of Science (2014): Indexed yes
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ISI indexed (2013): ISI indexed yes
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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
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Simulating X-ray telescopes with McXtrace: A case study of ATHENA’s optics

General information
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Organisations: National Space Institute, Astrophysics and Atmospheric Physics, Department of Physics, Neutrons and X-rays for Materials Physics, National Institute for Astrophysics, University of Copenhagen, European Space Agency
Authors: Della Monica Ferreira, D. (Intern), Bergbäck Knudsen, E. (Intern), Westergaard, N. J. S. (Intern), Christensen, F. E. (Intern), Massahi, S. (Intern), Shortt, B. (Ekstern), Spiga, D. (Ekstern), Solstade, M. (Ekstern), Lefmann, K. (Ekstern)
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ATHENA, Ray tracing, McXtrace, Simulation, X-rays, SPO, Effective area, Mirror module
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Simulation and modeling of silicon pore optics for the ATHENA X-ray telescope

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Article number: 99055O
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Simulation of neutrals in a turbulent scrape-off layer

General information
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Organisations: Department of Physics, Plasma Physics and Fusion Energy
Authors: Thrysøe, A. S. (Intern), Madsen, J. (Intern), Naulin, V. (Intern), Nielsen, A. H. (Intern), Juul Rasmussen, J. (Intern)
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Simulations of filamentary transport in the SOL and estimations of the power deposition profile

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Simulator of GAley Millimetre/submillimetre Emission (SiGAME): CO emission from massive z=2 main-sequence galaxies

We present SiGAME (SImulator of GAley Millimetre/submillimetre Emission), a new numerical code designed to simulate the $^{12}\text{CO}$ rotational line spectrum of galaxies. Using sub-grid physics recipes to post-process the outputs of smoothed particle hydrodynamics (SPH) simulations, a molecular gas phase is condensed out of the hot and partly ionized SPH gas. The gas is subjected to far-UV radiation fields and cosmic ray ionization rates which are set to scale with the local star formation rate volume density. Level populations and radiative transport of the CO lines are solved with the 3D radiative transfer code lime. We have applied SiGAME to cosmological SPH simulations of three disc galaxies at z = 2 with stellar masses in the range $0.5 - 2 \times 10^{11} M_{\odot}$ and star formation rates $40 - 140 M_{\odot}$ yr$^{-1}$. Global CO luminosities and line ratios are in agreement with observations of disc galaxies at z = 2 up to and including $J = 3 - 2$ but falling short of the few existing $J = 5 - 4$ observations. The central 5 kpc regions of our galaxies have CO 3 − 2 / 1 − 0 and 7 − 6 / 1 − 0 brightness temperature ratios of ~0.55−0.65 and ~0.02−0.08, respectively, while further out in the disc the ratios drop to more quiescent values of ~0.5 and ~0.01. Global CO-to-$H_2$ conversion ($\alpha_{\text{CO}}$) factors are $\approx 1.5 M_{\odot} pc^{-2}(K km s^{-1})^{-1}$, i.e. ~2−3 times below the typically adopted values for disc galaxies, and $\alpha_{\text{CO}}$ increases with radius, in agreement with observations of nearby galaxies. Adopting a top-heavy Giant Molecular Cloud (GMC) mass spectrum does not significantly change the results. Steepening the GMC density profiles leads to higher global line ratios for $J_{\text{up}} \geq 3$ and CO-to-$H_2$ conversion factors $\approx 3.6 M_{\odot} pc^{-2}(K km s^{-1})^{-1}$.

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Authors: Olsen, K. P. (Ekstern), Greve, T. R. (Ekstern), Brinch, C. (Intern), Sommer-Larsen, J. (Ekstern), Rasmussen, J. (Intern), Toft, S. (Ekstern), Zirm, A. (Ekstern)
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Simultaneous resonant x-ray diffraction measurement of polarization inversion and lattice strain in polycrystalline ferroelectrics

Structure-property relationships in ferroelectrics extend over several length scales from the individual unit cell to the macroscopic device, and with dynamics spanning a broad temporal domain. Characterizing the multi-scale structural origin of electric field-induced polarization reversal and strain in ferroelectrics is an ongoing challenge that so far has obscured its fundamental behaviour. By utilizing small intensity differences between Friedel pairs due to resonant scattering, we demonstrate a time-resolved X-ray diffraction technique for directly and simultaneously measuring both lattice strain and, for the first time, polarization reversal during in-situ electrical perturbation. This technique is demonstrated for BaTiO$_3$-BiZn$_{0.5}$Ti$_{0.5}$O$_3$ (BT-BZT) polycrystalline ferroelectrics, a prototypical lead-free piezoelectric with an ambiguous switching mechanism. This combines the benefits of spectroscopic and diffraction-based measurements into a single and robust technique with time resolution down to the ns scale, opening a new door to in-situ structure-property characterization that probes the full extent of the ferroelectric behaviour.

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Simultaneous resonant x-ray diffraction measurement of polarization inversion and lattice strain in polycrystalline ferroelectrics

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Scopus rating (2006): SJR 4.769 SNIP 1.326
Web of Science (2006): Indexed yes
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Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 3.104 SNIP 1.35
Scopus rating (2002): SJR 2.491 SNIP 1.325
Scopus rating (2001): SJR 2.251 SNIP 1.042
Web of Science (2001): Indexed yes
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Authors: Gorfman, S. (Ekstern), Simons, H. (Intern), Iamsasri, T. (Ekstern), Prasertpalichat, S. (Ekstern), Cann, D. P. (Ekstern), Choe, H. (Ekstern), Pietsch, U. (Ekstern), Watler, Y. (Ekstern), Jones, J. L. (Ekstern)
Number of pages: 9
Single-quadrature continuous-variable quantum key distribution

Most continuous-variable quantum key distribution schemes are based on the Gaussian modulation of coherent states followed by continuous quadrature detection using homodyne detectors. In all previous schemes, the Gaussian modulation has been carried out in conjugate quadratures thus requiring two independent modulators for their implementations. Here, we propose and experimentally test a largely simplified scheme in which the Gaussian modulation is performed in a single quadrature. The scheme is shown to be asymptotically secure against collective attacks, and considers a specific attack using asymmetric preparation and excess noise. We find that this protocol is considerably more sensitive to noise than other CVQKD schemes, as a consequence of the simplified implementation. A single-quadrature modulation approach renders the need for a costly amplitude modulator unnecessary, and thus facilitates commercialization of continuous-variable quantum key distribution, provided that the low noise requirement can be achieved.
In the present work, we have investigated the electrocatalytic activity of the oxygen reduction reaction (ORR), $\text{O}_2 + 4\text{H}^+ + 4e^- \rightarrow 2\text{H}_2\text{O}$, for (Pt$_n$) clusters ($n = 1, 2, 3, 5, 7, 10$ and $12$) adsorbed on semiconducting (2H) and metallic (1T) MoS$_2$ monolayers using first principles density functional theory. We have considered four elementary reactions involved in ORR within a unified electrochemical thermodynamic framework and the corresponding Gibbs adsorption free energies of the key intermediates (*OOH, *O, *OH) associated with each step have been calculated. The results indicate that the reduction of adsorbed hydroxyl (*OH) to water (*OH + H$^+$ + e$^-$ $\rightarrow$ H$_2$O) is the bottleneck step in the ORR process. The adsorption free energy of *OH ($\Delta G_{\text{ads}, \text{OH}}$) is found to be the thermodynamic descriptor for the present systems. Eventually, the ORR activity has been described as a function of $\Delta G_{\text{ads}, \text{OH}}$ and a volcano plot predicting (Pt)$_7$/2H-MoS$_2$ as the best ORR catalyst amongst the (Pt)$_n$/MoS$_2$ heterosystems with an overpotential value of 0.33 V has been established. Our finding proposes a new promising electrocatalyst towards better activity for ORR with very small amount of Pt loading.
Spin polarization in high density quark matter under a strong external magnetic field

In high density quark matter under a strong external magnetic field, possible phases are investigated by using the two-flavor Nambu-Jona-Lasinio (NJL) model with tensor-type four-point interaction between quarks, as well as the axial-vector-type four-point interaction. In the tensor-type interaction under the strong external magnetic field, it is shown that a quark spin polarized phase is realized in all regions of the quark chemical potential under consideration within the lowest Landau level approximation. In the axial-vector-type interaction, it is also shown that the quark spin polarized phase appears in the wide range of the quark chemical potential. In both the interactions, the quark mass in zero and small chemical potential regions increases which indicates that the chiral symmetry breaking is enhanced, namely the magnetic catalysis occurs.
Spin-polarized versus chiral condensate in quark matter at finite temperature and density

It is shown that the spin-polarized condensate appears in quark matter at high baryon density and low temperature due to the tensor-type four-point interaction in the Nambu-Jona-Lasinio-type model as a low-energy effective theory of quantum chromodynamics. It is indicated within this low-energy effective model that the chiral symmetry is broken again by the spin-polarized condensate on increasing the quark number density, while chiral symmetry restoration occurs, in which the
Stark shift and electric-field-induced dissociation of excitons in monolayer MoS$_2$ and hBN/MoS$_2$ heterostructures

Efficient conversion of photons into electrical current in two-dimensional semiconductors requires, as a first step, the dissociation of the strongly bound excitons into free electrons and holes. Here we calculate the dissociation rates and energy shift of excitons in monolayer MoS$_2$ as a function of an applied in-plane electric field. The dissociation rates are obtained as the inverse lifetime of the resonant states of a two-dimensional hydrogenic Hamiltonian which describes the exciton within the Mott-Wannier model. The resonances are computed using complex scaling, and the effective masses and screened electron-hole interaction defining the hydrogenic Hamiltonian are computed from first principles. For field strengths above 0.1 V/nm the dissociation lifetime is shorter than 1 ps, which is below the lifetime associated with competing decay mechanisms. Interestingly, encapsulation of the MoS$_2$ layer in just two layers of hexagonal boron nitride (hBN), enhances the dissociation rate by around one order of magnitude due to the increased screening. This shows that dielectric engineering is an effective way to control exciton lifetimes in two-dimensional materials.
Stomatal design principles in synthetic and real leaves

Stomata are portals in plant leaves that control gas exchange for photosynthesis, a process fundamental to life on Earth. Gas fluxes and plant productivity depend on external factors such as light, water and CO2 availability and on the geometrical properties of the stoma pores. The link between stoma geometry and environmental factors has informed a wide range of scientific fields—from agriculture to climate science, where observed variations in stoma size and density are used to infer prehistoric atmospheric CO2 content. However, the physical mechanisms and design principles responsible for major trends in stomatal patterning are not well understood. Here, we use a combination of biomimetic experiments and theory to rationalize the observed changes in stoma geometry. We show that the observed correlations between stoma size and density are consistent with the hypothesis that plants favour efficient use of space and maximum control of dynamic gas conductivity, and that the capacity for gas exchange in plants has remained constant over at least the last 325 Myr. Our analysis provides a new measure to gauge the relative performance of species based on their stomatal characteristics.
Structural dynamics of solvated metal complexes with anisotropy-enhanced X-ray scattering

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Authors: Biasin, E. (Intern), Nielsen, M. M. (Intern), Haldrup, K. (Intern)
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Structure-activity investigation of Ni-Ga model catalysts for CO$_2$ hydrogenation to Methanol

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Structure – Activity – Stability Relationship of Nanostructured Model Electrodes

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Studying a bifunctional Cu/ZnO-zeolite catalyst for direct production of dimethyl ether with in situ ptychography and ETEM

**General information**
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Organisations: Center for Electron Nanoscopy, Department of Physics, Experimental Surface and Nanomaterials Physics, Karlsruhe Institute of Technology KIT, Deutsches Elektronensynchrotron DESY, Friedrich-Alexander University Erlangen-Nuremberg, University of Hamburg
Authors: Baier, S. (Ekstern), Damsgaard, C. D. (Intern), Reinhardt, J. (Ekstern), Klumpp, M. (Ekstern), Benzi, F. (Ekstern), Scholz, M. (Ekstern), Sheppard, T. (Ekstern), Balogh, Z. I. (Intern), Kasama, T. (Intern), Wagner, J. B. (Intern), Schwieger, W. (Ekstern), Schroer, C. (Ekstern), Grunwaldt, J. (Ekstern)
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Study on the L–H transition power threshold with RF heating and lithium-wall coating on EAST
The power threshold for low (L) to high (H) confinement mode transition achieved by radio-frequency (RF) heating and lithium-wall coating is investigated experimentally on EAST for two sets of walls: an all carbon wall (C) and molybdenum chamber and a carbon divertor (Mo/C). For both sets of walls, a minimum power threshold $P_{\text{thr}}$ of $\sim 0.6$ MW was found when the EAST operates in a double null (DN) divertor configuration with intensive lithium-wall coating. When operating in upper single null (USN) or lower single null (LSN), the power threshold depends on the ion $\nabla B$ drift direction. The low density dependence of the L–H power threshold, namely an increase below a minimum density, was identified in the Mo/C wall for the first time. For the C wall only the single-step L–H transition with limited injection power is observed whereas also the so-called dithering L–H transition is observed in the Mo/C wall. The dithering behaves distinctively in a USN, DN and LSN configuration, suggesting the divertor pumping capability is an important ingredient in this transition since the internal cryopump is located underneath the lower divertor. Depending on the chosen divertor configuration, the power across the separatrix $P_{\text{loss}}$ increases with neutral density near the lower X-point in EAST with the Mo/C wall, consistent with previous results in the C wall (Xu et al 2011 Nucl. Fusion 51 072001). These findings suggest that the edge neutral density, the ion $\nabla B$ drift as well as the divertor pumping capability play important roles in the L–H power threshold and transition behaviour.

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Organisations: Department of Physics, Plasma Physics and Fusion Energy, Chinese Academy of Sciences
Authors: Chen, L. (Ekstern), Xu, G. (Ekstern), Nielsen, A. H. (Intern), Gao, W. (Ekstern), Duan, Y. (Ekstern), Liu, H. (Ekstern), Wang, L. (Ekstern), Li, M. (Ekstern), Wang, M. (Ekstern), Zhang, X. (Ekstern), Chen, R. (Ekstern), Wang, H. (Ekstern), Sun, Z. (Ekstern), Ding, S. (Ekstern), Yan, N. (Ekstern), Liu, S. (Ekstern), Shao, L. (Ekstern), Zhang, W. (Ekstern), Hu, G. (Ekstern), Li, J. (Ekstern), Zhang, L. (Ekstern), Wan, B. (Ekstern)
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Main Research Area: Technical/natural sciences

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Superconducting Dy1-x(Gd,Yb)Ba2Cu3O7-δ thin films made by Chemical Solution Deposition

Dy1-x(Gd or Yb)Ba2Cu3O7-δ 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_{onset}) were found to decrease with increasing Yb content, while only minor changes were observed for samples with Gd. Critical current density (Jc) analysis demonstrated that doping with Yb significantly increased the self-field Jc value from 3.8 MA/cm² to 6.0 MA/cm² for the pure and 10 % Yb doped sample, respectively. In contrast, samples doped with Gd were characterized by the lowest self-field Jc values. Investigation of pinning force mechanisms revealed that the samples in this study were dominated by normal surface pinning.

General information

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Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Department of Physics, Quantum Physics and Information Technology
Authors: Opata, Y. A. (Intern), Wulff, A. C. (Intern), Hansen, J. O. B. (Ekstern), Yue, Z. (Intern), Grivel, J. (Intern)
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Scopus rating (2015): SJR 0.403 SNIP 1.06 CiteScore 1.27
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Superhydrophobic Properties of Nanotextured Polypropylene Foils Fabricated by Roll-to-Roll Extrusion Coating

We demonstrate the use of roll-to-roll extrusion coating (R2R-EC) for fabrication of nanopatterned polypropylene (PP) foils with strong antitwetting properties. The antitwetting nanopattern is originated from textured surfaces fabricated on silicon wafers by a single-step method of reactive ion etching with different processing gas flow rates. We provide a systematic study of the wetting properties for the fabricated surfaces and show that a controlled texture stretching effect in the R2R-EC process is instrumental to yield the superhydrophobic surfaces with water contact angles approaching 160° and droplet roll-off angles below 10°.

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Organisations: Department of Micro- and Nanotechnology, Polymer Micro & Nano Engineering, Department of Photonics Engineering, Optical Microsystems and Micromaterials, Department of Physics, Risø National Laboratory for Sustainable Energy, Inmold A/S
Authors: Telecka, A. (Intern), Murthy, S. (Intern), Sun, L. (Intern), Pranov, H. (Ekstern), Taboryski, R. J. (Intern)
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Main Research Area: Technical/natural sciences

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Support effect on the activity and thermal stability of platinum nanoparticles for diesel oxidation

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Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2016

Sustainable Electrochemical Hydrogen Production
Molecular hydrogen (H₂) is one of the world’s most important chemicals with a global production rate of approximately 50 billion kg per year. Today hydrogen is mainly used for petroleum refining and for synthesizing ammonia-based fertilizers but hydrogen also hold promise for the transportation sector using fuel cell vehicles. As hydrogen is mainly produced from fossil fuels, developing an alternative, renewable pathway to produce H₂ in a cost-competitive manner would have a significant impact in reducing fossil fuel consumption and CO₂ emissions. One attractive pathway for clean hydrogen production is through electrochemical processes coupled to renewable energy sources such as wind or solar.

The hydrogen evolution reaction (HER, 2H⁺ + 2e⁻ → H₂) constitutes half of the water splitting reaction. To increase process efficiency, active catalysts for the HER are needed. Currently platinum is the best known HER catalyst as only small overpotentials are required to drive high reaction rates, but the scarcity and high cost of Pt may limit its widespread technological use. This has sparked a search for Earth-abundant catalysts that potentially could replace Pt - a search where the development of molybdenum sulfide (MoS₂)-based HER catalysts serves as an excellent example of theory-guided discovery and design of new electrocatalysts.”
For decades, MoS$_2$ was believed to be inactive for the HER. However, inspired by hydrogen-producing enzymes such as hydrogenase and nitrogenase in nature, theoretical calculations predicted the edges of MoS$_2$ layers to be active. Guided by these calculations, several nanostructured MoS$_2$ catalysts have been synthesized to expose edge sites. In my talk, I will show this extraordinary development of non-precious metal HER catalysts and highlight a specific example of one such catalyst; [Mo$_3$S$_{13}$]$^{2-}$ nanoclusters.

**General information**

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Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics, Stanford University

Authors: Kibsgaard, J. (Intern), Jaramillo, T. F. (Ekstern), Chorkendorff, I. (Intern)

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**Bibliographical note**

Sustain Abstract P-2

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**Synthesis of ligand-free CZTS nanoparticles via a facile hot injection route**

Single-phase, ligand-free Cu$_2$ZnSnS$_4$ (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**

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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)

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Web of Science (2016): Indexed yes
Tailoring Mixed-Halide, Wide-Gap Perovskites via Multistep Conversion Process

Wide-band-gap mixed-halide CH$_3$NH$_3$Pb$_{1-x}$Br$_x$-based solar cells have been prepared by means of a sequential spin-coating process. The spin-rate for PbI$_2$, as well as its repetitive deposition, are important in determining the cross-sectional shape and surface morphology of perovskite, and, consequently, J–V performance. A perovskite solar cell converted from PbI$_2$ with a dense bottom layer and porous top layer achieved higher device performance than those of analogue cells with a dense PbI$_2$ top layer. This work demonstrates a facile way to control PbI$_2$ film configuration and morphology simply by modification of spin-coating parameters without any additional chemical or thermal post-treatment.
Targeted design of α-MnO₂ based catalysts for oxygen reduction

The paper focuses on theoretical and experimental aspects of an oxide surface optimization for oxygen reduction reaction (ORR). Various doped α-MnO₂ based electrocatalysts were prepared by microwave-assisted hydrothermal synthesis and electrochemically characterized to validate density functional theory (DFT) based predictions of the oxidation state and local structure effects on the catalytic activity of α-MnO₂ catalysts in ORR. Both theory and experiments conclude that the highest activity in ORR is to be expected in the case of clustered Mn³⁺ sites which yield activity comparable with that of the polycrystalline Pt. These active sites have to be formed under in-operando conditions and their formation is hindered in doped alpha-MnO₂ catalysts. The activity of the other conceivable active sites based on non-clustered Mn³⁺ or Mn⁴⁺ is inferior to that of clustered Mn³⁺. The activation of Mn³⁺ or Mn⁴⁺ based active sites leads to a shift in selectivity of the ORR process towards 2 electron formation of hydrogen peroxide.

General information

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Organisations: Center for Atomic-scale Materials Design, Department of Physics, Academy of Sciences of the Czech Republic, University of Copenhagen
Authors: Lehtimaeki, M. (Ekstern), Hoffmannova, H. (Ekstern), Boytsova, O. (Ekstern), Bastl, Z. (Ekstern), Busch, M. (Intern), Halck, N. B. (Intern), Rossmeisl, J. (Ekstern), Krtil, P. (Ekstern)
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Web of Science (2016): Indexed yes
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BFI (2014): BFI-level 2
Temperature dependent piezoelectric response and strain-electric-field hysteresis of rare-earth modified bismuth ferrite ceramics

The rare-earth (RE)-modified bismuth ferrite (BiFeO₃ or BFO) family of ferroelectrics have uncomplicated lead-free chemistries and simple perovskite structures. Due to the high Curie transition temperature of the parent BiFeO₃ perovskite (similar to 830 °C), they are promising piezoelectric materials for use at elevated temperatures. However, the influence of the specific RE species on the electromechanical behavior at high temperatures and above the coercive electric-field is not widely reported. Here, structural analysis over multiple length scales using X-ray diffraction, transmission electron microscopy and piezoresponse force microscopy is coupled with a high electric-field cycling study and in situ converse d³₃ measurements up to 325 °C for three RE-BFO ceramic compositions, Bi₀.₈₆Sm₀.₁₄FeO₃, Bi₀.₈₈Gd₀.₁₂FeO₃ and Bi₀.₉₁Dy₀.₀₉FeO₃. The ceramics exhibit different phase assemblages with varying amounts of polar rhombohedral R3c and intermediate antipolar orthorhombic Pbam phases as a function of the RE species. During electric-field cycling at electric-
fields with amplitudes of 160 kV cm\(^{-1}\), peak-to-peak strains of 0.23-0.27% are reached for all three compositions. However, there are qualitative differences in the field-induced strain and electric current behavior as a function of electric-field cycling and the materials exhibit an electrical-history dependent behavior. \(\text{Bi}_{0.91}\text{Dy}_{0.09}\text{FeO}_3\) possesses an improved \(d_{33}\) stability as a function of temperature relative to the parent BFO perovskite and the highest depolarization temperature among the three RE-BFO compositions, with a stable \(d_{33}\) of similar to 22 pC N\(^{-1}\) up to 325 °C.

**General information**

State: Published

Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Josef Stefan Institute, University of Sheffield, University of New South Wales, Politecnico di Torino

Authors: Walker, J. (Ekstern), Ursic, H. (Ekstern), Bencan, A. (Ekstern), Malic, B. (Ekstern), Simons, H. (Intern), Reaney, I. (Ekstern), Viola, G. (Ekstern), Nagarajan, V. (Ekstern), Rojac, T. (Ekstern)

Number of pages: 10

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Publication date: 2016

Main Research Area: Technical/natural sciences

**Publication information**

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Volume: 4

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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

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Publication: Research - peer-review › Journal article – Annual report year: 2016

**Temperature dynamics and velocity scaling laws for interchange driven, warm ion plasma filaments**

The influence of electron and ion temperature dynamics on the radial convection of isolated structures in magnetically confined plasmas is investigated by means of numerical simulations. It is demonstrated that the maximum radial velocity of these plasma blobs roughly follows the inertial velocity scaling, which is proportional to the ion acoustic speed times the square root of the filament particle density times the sum of the electron and ion temperature perturbations. Only for small blobs the cross field convection does not follow this scaling. The influence of finite Larmor radius effects on the cross-field blob convection is shown not to depend strongly on the dynamical ion temperature field. The blob dynamics of constant finite and dynamical ion temperature blobs is similar. When the blob size is on the order of 10 times the ion Larmor radius the blobs stay coherent and decelerate slowly compared to larger blobs which dissipate faster due to fragmentation and turbulent mixing.

**General information**

State: Published
Temlated green synthesis of plasmonic silver nanoparticles in onion epidermal cells suitable for surface-enhanced Raman and hyper-Raman scattering

We report fast and simple green synthesis of plasmonic silver nanoparticles in the epidermal cells of onions after incubation with AgNO₃ solution. The biological environment supports the generation of silver nanostructures in two ways. The plant tissue delivers reducing chemicals for the initial formation of small silver clusters and their following conversion to plasmonic particles. Additionally, the natural morphological structures of the onion layers, in particular the extracellular matrix provides a biological template for the growth of plasmonic nanostructures. This is indicated by red glowing images of extracellular spaces in dark field microscopy of onion layers a few hours after AgNO₃ exposure due to the formation of silver nanoparticles. Silver nanostructures generated in the extracellular space of onion layers and within the epidermal cell walls can serve as enhancing plasmonic structures for one-and two-photon-excited spectroscopy such as surface enhanced Raman scattering (SERS) and surface enhanced hyper-Raman scattering (SEHRS). Our studies demonstrate a templated green preparation of enhancing plasmonic nanoparticles and suggest a new route to deliver silver nanoparticles as basic building blocks of plasmonic nanosensors to plants by the uptake of solutions of metal salts.

General information
State: Published
Organisations: Department of Physics, Biophysics and Fluids, Department of Micro- and Nanotechnology, Humboldt-Universität zu Berlin
Authors: Palanco, M. E. (Intern), Mogensen, K. B. (Intern), Guehlke, M. (Ekstern), Heiner, Z. (Ekstern), Kneipp, J. (Ekstern), Kneipp, K. (Intern)
Number of pages: 7
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Main Research Area: Technical/natural sciences

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BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 1.233 SJR 1.119 CiteScore 3.32
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.86 SJR 1.138 SNIP 1.026
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.001 SNIP 0.944 CiteScore 3.05
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.163 SNIP 1.038 CiteScore 2.67
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.268 SNIP 1.057 CiteScore 2.56

Scopus rating (2002): SJR 1.668 SNIP 1.058
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 1.679 SNIP 1.233
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 1.974 SNIP 1.097
Scopus rating (1999): SJR 2.001 SNIP 1.471
Original language: English
Velocity scaling, Warm ions, Scrape-off layer transport, Blob dynamics
DOI:
10.1088/0741-3335/58/4/044011
Source: FindIt
Source-ID: 2292431255
Publication: Research - peer-review › Journal article – Annual report year: 2016
Testing the Münch hypothesis of long distance phloem transport in plants

Long distance transport in plants occurs in sieve tubes of the phloem. The pressure flow hypothesis introduced by Ernst Münch in 1930 describes a mechanism of osmotically generated pressure differentials that are supposed to drive the movement of sugars and other solutes in the phloem, but this hypothesis has long faced major challenges. The key issue is whether the conductance of sieve tubes, including sieve plate pores, is sufficient to allow pressure flow. We show that with increasing distance between source and sink, sieve tube conductivity and turgor increases dramatically in Ipomoea nil. Our results provide strong support for the Münch hypothesis, while providing new tools for the investigation of one of the least understood plant tissues.
The effect of inter-granular constraints on the response of polycrystalline piezoelectric ceramics at the surface and in the bulk

The electro-mechanical coupling mechanisms in polycrystalline ferroelectric materials, including a soft PbZr\textsubscript{x}Ti\textsubscript{1-x}O\textsubscript{3} (PZT) and lead-free 0.9375(Bi\textsubscript{1/2}Na\textsubscript{1/2})TiO\textsubscript{3}-0.0625BaTiO\textsubscript{3} (BNT-6.25BT), have been studied using a surface sensitive low-energy (12.4 keV) and bulk sensitive high-energy (73 keV) synchrotron X-ray diffraction with in situ electric fields. The results show that for tetragonal PZT at a maximum electric field of 2.8 kV/mm, the electric-field-induced lattice strain ($\varepsilon_{111}$) is 20% higher at the surface than in the bulk, and non-180° ferroelectric domain texture (as indicated by the intensity ratio $I_{002}/I_{200}$) is 16% higher at the surface. In the case of BNT-6.25BT, which is pseudo-cubic up to fields of 2 kV/mm, lattice strains $\varepsilon_{111}$ and $\varepsilon_{200}$ are 15% and 20% higher at the surface, while in the mixed tetragonal and rhombohedral phases at 5 kV/mm, the domain texture indicated by the intensity ratio $I_{111}/I_{111\bar{1}}$ and $I_{002}/I_{200}$ are 12% and 10% higher at the surface than in the bulk, respectively. The observed difference in the strain contributions between the surface and bulk is suggested to result from the fact that surface grains are not constrained in three dimensions, and consequently, domain reorientation and lattice expansion in surface grains are promoted. It is suggested that the magnitude of property difference between the surface and bulk is higher for the PZT than for BNT-6.25BT due to the level of anisotropy in the strain mechanism. The comparison of the results from different methods demonstrates that the intergranular constraints have a significant influence on the electric-field-induced electro-mechanical responses in polycrystalline ferroelectrics. These results have implications for the design of higher performance polycrystalline piezoelectrics.
The influence of blobs on neutral particles in the scrape-off layer

Interactions between plasma and neutrals are investigated with particular attention to the influence of large amplitude blob structures that mediate a significant particle and energy transport through the scrape-off layer (SOL). We perform a statistical analysis of the mean-field approximation for plasma parameters in the SOL, and this approximation is shown to be poor in a SOL with a high level of fluctuations, as the plasma fields are strongly correlated. A 1D neutral fluid model
which account for both cold and hot neutrals is formulated and the effects of blobs on the ionization in the SOL and edge are investigated. Simulations suggest that neutrals originating from dissociation of hydrogen molecules only fuel in the outermost edge region of the plasma, whereas hot neutrals from charge exchange collisions penetrate deep into the bulk plasma. The results are recovered in a simplified 2D model.

General information
State: Published
Organisations: Department of Physics, Plasma Physics and Fusion Energy
Authors: Thrysøe, A. S. (Intern), Tophøj, L. E. H. (Intern), Naulin, V. (Intern), Rasmussen, J. J. (Intern), Madsen, J. (Intern)
Nielsen, A. H. (Intern)
Number of pages: 9
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Plasma Physics and Controlled Fusion
Volume: 58
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BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 1.243 SJR 0.69 CiteScore 1.74
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1 SJR 1.433 SNIP 1.258
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.314 SNIP 1.345 CiteScore 1.1
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.542 SNIP 1.346 CiteScore 1.61
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.2 SNIP 1.253 CiteScore 1.54
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.453 SNIP 1.201 CiteScore 1.63
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.496 SNIP 1.591 CiteScore 2.69
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.468 SNIP 1.408
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.589 SNIP 1.324
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.845 SNIP 1.569
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.927 SNIP 1.374
The influence of electrodialytic remediation on dioxin (PCDD/PCDF) levels in fly ash and air pollution control residues

Fly ash and Air Pollution Control (APC) residues collected from three municipal solid waste incinerators in Denmark and Greenland were treated by electrodialytic remediation at pilot scale for 8-10 h. This work presents for the first time the effect of electrodialytic treatment on polychlorinated dibenzo-p-dioxins (PCDD) and polychlorinated dibenzofurans (PCDF), and how these levels impact on the valorization options for fly ash and APC residue. PCDD/PCDF levels in the original residues ranged between 4.85 and 197 ng g⁻¹, being higher for the electrostatic precipitator fly ash. The toxic equivalent (TEQ) varied ten fold, ranging 0.18-2.0 ng g⁻¹ I-TEQ with penta and hexa-homologs being most significant for toxicity. After the electrodialytic treatment PCDD/PCDF levels increased in the residues (between 1.4 and 2.0 times). This does not mean PCDD/PCDF were synthesized, but else that soluble materials dissolve, leaving behind the non-water soluble compounds, such as PCDD/PCDF. According to the Basel Convention, PCDD/PCDF levels in these materials is low (<15 mg WHO-TEQ kg⁻¹) and the fly ash and APC residue could eventually be valorized, for instance as construction material, provided end-of-waste criteria are set and that a risk assessment of individual options is carried out, including the end-of-life stage when the materials become waste again.

General information
State: Published
Organisations: Department of Civil Engineering, ARTEK, Section for Arctic Engineering and Sustainable Solutions, Department of Physics, Aveiro University
Authors: Dias-Ferreira, C. (Ekstern), Kirkelund, G. M. (Intern), Jensen, P. E. (Intern)
Number of pages: 8
Pages: 380-387
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Chemosphere
Volume: 148
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Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): SJR 1.435 SNIP 1.447 CiteScore 4.62
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.39 SJR 1.447 SNIP 1.625
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
The influence of temperature dynamics and dynamic finite ion Larmor radius effects on seeded high amplitude plasma blobs

Thermal effects on the perpendicular convection of seeded pressure blobs in the scrape-off layer of magnetised fusion plasmas are investigated. Our numerical study is based on a four field full-F gyrofluid model, which entails the consistent description of high fluctuation amplitudes and dynamic finite Larmor radius effects. We find that the maximal radial blob velocity increases with the square root of the initial pressure perturbation and that a finite Larmor radius contributes to highly compact blob structures that propagate in the poloidal direction. An extensive parameter study reveals that a smooth transition to this compact blob regime occurs when the finite Larmor radius effect strength, defined by the ratio of the magnetic field aligned component of the ion diamagnetic to the $E \times B$ vorticity, exceeds unity. The maximal radial blob velocities agree excellently with the inertial velocity scaling law over more than an order of magnitude. We show that the finite Larmor radius effect strength affects the poloidal and total particle transport and present an empirical scaling law for the poloidal and total blob velocities. Distinctions to the blob behaviour in the isothermal limit with constant finite Larmor radius effects are highlighted.
The negative piezoelectric effect of the ferroelectric polymer poly(vinylidene fluoride)

Piezoelectricity describes interconversion between electrical charge and mechanical strain. As expected for lattice ions displaced in an electric field, the proportionality constant is positive for all piezoelectric materials. The exceptions are poly(vinylidene fluoride) (PVDF) and its copolymers with trifluoroethylene (P(VDF-TrFE)), which exhibit a negative longitudinal piezoelectric coefficient. Reported explanations exclusively consider contraction with applied electric field of either the crystalline or the amorphous part of these semi-crystalline polymers. To distinguish between these conflicting interpretations, we have performed in situ dynamic X-ray diffraction measurements on P(VDF-TrFE) capacitors. We find that the piezoelectric effect is dominated by the change in lattice constant but, surprisingly, it cannot be accounted for by the polarization-biased electrostrictive contribution of the crystalline part alone. Our quantitative analysis shows that an
additional contribution is operative, which we argue is due to an electromechanical coupling between the intermixed crystalline lamellae and amorphous regions. Our findings tie the counterintuitive negative piezoelectric response of PVDF and its copolymers to the dynamics of their composite microstructure.

**General information**

State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Max Planck Institute for Polymer Research, University of Groningen, Swiss Federal Institute of Technology
Pages: 78-84
Publication date: 2016
Main Research Area: Technical/natural sciences

**Publication information**

Journal: Nature Materials
Volume: 15
Issue number: 1
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
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 18.482 SNIP 8.331 CiteScore 21.29
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 17.79 SNIP 7.876 CiteScore 19.84
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 18.404 SNIP 7.654
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
Scopus rating (2007): SJR 10.274 SNIP 5.685
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: 2016

Thermal decomposition of ammonium hexachloroosmate

Structural changes of (NH₄)₂[OsCl₆] occurring during thermal decomposition in a reduction atmosphere have been studied in situ using combined energy-dispersive X-ray absorption spectroscopy (ED-XAFS) and powder X-ray diffraction (PXRD). According to PXRD, (NH₄)₂[OsCl₆] transforms directly to metallic Os without the formation of any crystalline intermediates but through a plateau where no reactions occur. XANES and EXAFS data by means of Multivariate Curve Resolution (MCR) analysis show that thermal decomposition occurs with the formation of an amorphous intermediate {OsCl₄}ₓ with a possible polymeric structure. Being revealed for the first time the intermediate was subjected to determine the local atomic structure around osmium. The thermal decomposition of hexachloroosmate is much more complex and occurs within a minimum two-step process, which has never been observed before.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, RAS - Nikolaev Institute of Inorganic Chemistry of SB, Novosibirsk State University, Swansea University
Authors: Asanova, T. I. (Ekstern), Kantor, I. (Intern), Asanov, I. P. (Ekstern), Korenev, S. V. (Ekstern), Yusenko, K. V. (Ekstern)
Number of pages: 8
Pages: 33134-33141
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
The test beamline of the European Spallation Source - Instrumentation development and wavelength frame multiplication

The European Spallation Source (ESS), scheduled to start operation in 2020, is aiming to deliver the most intense neutron beams for experimental research of any facility worldwide. Its long pulse time structure implies significant differences for instrumentation compared to other spallation sources which, in contrast, are all providing short neutron pulses. In order to enable the development of methods and technology adapted to this novel type of source well in advance of the first instruments being constructed at ESS, a test beamline (TBL) was designed and built at the BER II research reactor at Helmholtz-Zentrum Berlin (HZB). Operating the TBL shall provide valuable experience in order to allow for a smooth start of operations at ESS. The beamline is capable of mimicking the ESS pulse structure by a double chopper system and provides variable wavelength resolution as low as 0.5% over a wide wavelength band between 1.6 A and 10 A by a dedicated wavelength frame multiplication (WFM) chopper system. WFM is proposed for several ESS instruments to allow for flexible time-of-flight resolution. Hence, ESS will benefit from the TBL which offers unique possibilities for testing methods and components. This article describes the main capabilities of the instrument, its performance as experimentally verified during the commissioning, and its relevance to currently starting ESS instrumentation projects.
The Villum Center for the Science of Sustainable Fuels and Chemicals

The research of the VILLUM Center focuses on solving two of the major challenges in order to meet the political objective of achieving a fossil-free society by 2050. The transition from fossil fuels to renewable energy sources call for:

1. More efficient storage of renewable energy
2. Viable alternatives to chemicals, plastics and other materials which are currently produced by using oil and coal—as well as finding alternatives to fossil-based fuels for aircraft, for example, which cannot be electrified and thus exploit renewable energy.

The key to both challenges is to develop better catalysts to promote the various chemical processes. The center will develop a systematic methodology to accelerate the discovery process for new catalysts. It will do that in a concerted effort, which is composed of six interdependent sub-projects closely interlinked.

Denmark is the international leader within both catalyst research and production. The research center hopes to achieve a research breakthrough in the area, which in turn can pave the way for further technological development ensuring that the exploitation of renewable energy in future will be so efficient that it can compete with fossil fuels and in the long term completely replace them.

General information
State: Published
Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics
Authors: Nielsen, J. H. (Intern)
Number of pages: 1
Publication date: 2016
Main Research Area: Technical/natural sciences
Links:
Three Things in one go - Heritage, Research and Dissemination at the Technical University of Denmark.

General information
State: Published
Organisations: Department of Physics
Authors: Zwisler, L. (Intern)
Pages: 209-222
Publication date: 2016

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Title of host publication: Enhancing University Heritage-Based Research: Proceedings of the XV Universeum Network Meeting, Hamburg, 12–14 June 2014
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Chapter: 19
Series: Nuncius Hamburgensis – Beiträge zur Geschichte der Naturwissenschaften
Volume: 33
ISSN: 1610-6164
Main Research Area: Technical/natural sciences
Conference: XV Universeum Network Meeting, Hamburg, Germany, 12/06/2014 - 12/06/2014
Source: PublicationPreSubmission
Source-ID: 125494453
Publication: Research - peer-review › Article in proceedings – Annual report year: 2016

Three-wave interaction during electron cyclotron resonance heating and current drive
Non-linear wave-wave interactions in fusion plasmas, such as the parametric decay instability (PDI) of gyrotron radiation, can potentially hamper the use of microwave diagnostics. Here we report on anomalous scattering in the ASDEX Upgrade tokamak during electron cyclotron resonance heating experiments. The observations can be linked to parametric decay of the gyrotron radiation at the second harmonic upper hybrid resonance layer.

General information
State: Published
Organisations: Department of Physics, Plasma Physics and Fusion Energy, Technical University of Denmark, Max-Planck-Institut fur Plasmaphysik
Number of pages: 2
Publication date: 2016

Host publication information
Title of host publication: 2016 41st International Conference on Infrared, Millimeter, and Terahertz waves
Publisher: IEEE
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ISBN (Electronic): 978-1-4673-8485-8
Series: International Conference on Infrared, Millimeter and Terahertz Waves
ISSN: 2162-2027
Main Research Area: Technical/natural sciences
DOIs: 10.1109/IRMMW-THz.2016.7758400
Source: FindIt
Source-ID: 2349437031
Publication: Research - peer-review › Article in proceedings – Annual report year: 2016
**Time-of-flight 3D Neutron Diffraction for Multigrain Crystallography**

This thesis presents a new technique for measuring spatially resolved microstructures in crystalline materials using pulsed neutron beams. The method, called Time-of-Flight Three Dimensional Neutron Diffraction (ToF 3DND), identifies the position, shape and crystallographic orientation of the individual grains within the sample. The experiments were conducted at the single crystal diffractometer SENJU at the Japanese neutron source J-PARC. The choice of this instrument was motivated by its large coverage of the reciprocal space.

The instrument had to undergo modifications to enable ToF 3DND measurements: a time resolved imaging detector, developed at University of Berkeley, California, was fitted in the interior of SENJU in order to record the extinction spots in the transmitted beam (i.e. areas with missing intensity due to Bragg diffraction of the individual grains).

The arrangement of the two detector systems facilitated two versions of ToF 3DND. The first version, restricted to imaging data, enables reconstruction of the position and shape of the individual grains without the use of crystallography. Afterwards, the orientations of the individual grains are indexed. The algorithms for both steps have been developed in this study. The work also shows that based on the transmission data alone the orientations are not uniquely determined; however, it is possible to find an unique solution by including diffraction signals from the imaging detector. The second version uses an existing method for indexing SENJU data, which then serves as prior information to restrict the extinction spots that belong to the same grain.

The ToF 3DND methods are verified through the study of two different samples: an Iron rod and a shape memory alloy (SMA) CoNiGa bi-crystal. Part of this verification involves comparison with electron backscatter diffraction (EBSD). In the Iron rod, 107 grains were indexed from the SENJU data. As a comparison, 108 grains were reconstructed from the nearfield data alone. This constitutes roughly 10 times as many grains as previously reported using a continuous neutron source.

Thanks to the penetrating properties of the neutron, ToF 3DND complements existing X-ray techniques in those cases where X-rays cannot penetrate the sample. Besides, with ToF 3DND it is also much easier to detect light elements such as those in energy materials.

With a future availability of an energy dispersive x-ray detector with high energy resolution, the methods reported here can be directly transferred to synchrotron and white beam based studies.

**General information**

**State:** Published  
**Organisations:** Department of Physics, Neutrons and X-rays for Materials Physics  
**Authors:** Cereser, A. (Intern), Hall, S. A. (Ekstern), Steuwer, A. (Ekstern), Strobl, M. (Ekstern), Schmidt, S. (Intern)  
**Number of pages:** 152  
**Publication date:** 2016

**Publication information**  
**Publisher:** Department of Physics, Technical University of Denmark  
**Original language:** English  
**Main Research Area:** Technical/natural sciences  
**Electronic versions:** Thesis_3DND..pdf

**Relations**  
**Projects:**  
Time-of-flight 3D Neutron Diffraction for Multigrain Crystallography  
**Publication:** Research › Ph.D. thesis – Annual report year: 2016

**Topology Optimized Components for Mode- and Wavelength Division Multiplexing**

This thesis deals with the topic of passive integrated nanophotonic devices realized in silicon on insulator material. The project has been concerned with all the steps of the process: Design, fabrication and characterization. The focus has been on using the inverse design method topology optimization. The method has been employed extensively to obtain various nanophotonic components. One of the outcomes of the project has been the development of a solid understanding of the benefits and limitations of topology optimization. This thesis presents numerous designs that have been characterized both through simulations and experiments. Among these are converters and (de-)multiplexers for mode division multiplexing, both realized with a record small footprint. Wavelength multiplexing devices were used as a basis for investigating the correlation between structure sizes and performance. Fortunately a larger footprint does not always give rise to better performance, however allowing for smaller feature sizes will. The design of compact tapers was commenced. Difficulties were met when working with very wide waveguides but methods for overcoming these were suggested. A novel form of cladding modulated Bragg gratings, utilizing continuous rails to modify the refractive index and cause the reflections, has also been proposed and experimentally verified as part of this project. This work has contributed additional components to the toolbox of devices necessary for integrated photonics. It has been shown that topology optimization is a strong method for creating extremely compact devices, the small features do however mean that they are not yet possible to fabricate on a large scale. Complex device functionalities can be obtained. Building on previous work of simpler structures it is comparatively easy to remake the new designs and then increase complexity without much impact on the footprint. The benefit of inverse design tools, like topology optimization, is that they lead to structures without geometrical constraints and which are independent of the designer. This project has however shown, that the best results are obtained when iterating on the optimized structures and providing the tool with well-chosen starting point structures.
Toward Molecular Magnets of Organic Origin via Anion-π Interaction Involving m-Aminyl Diradical: A Theoretical Study

Here we study a set of novel magnetic organic molecular species with different halide ions (fluoride, chloride, bromide) absorbed ~2 Å above or below the center of an aromatic π-ring in an m-aminyl diradical. Focus is on the nature of anion-π interaction and its impact on magnetic properties, specifically on magnetic anisotropy and on intramolecular magnetic exchange coupling. In the development of single molecule magnets, magnetic anisotropy is considered to be the most influential factor. A new insight regarding the magnetic anisotropy that determines the barrier height for relaxation of magnetization of m-aminyl diradical-derived anionic complexes is obtained from calculations of the axial zero-field-splitting (ZFS) parameter D. The noncovalent anion-π interaction strongly influences magnetic anisotropy in m-aminyl-halide diradical complexes. In particular, the change of D values from positive (for the m-aminyl diradical, m-aminyl diradical/fluoride, and m-aminyl diradical/chloride complexes) to negative D-values in m-aminyl diradical complexes containing bromide signals a change from oblate to prolate type of spin-density distribution. Furthermore, the noncovalent halide-π interactions lead to large values of intramolecular magnetic exchange coupling coefficients J exhibiting a ferromagnetic sign. The magnitude of J steadily increases going from anionic complexes containing fluoride to chloride and then to bromide. Relations are sought between the magnetic exchange coupling coefficients J and aromaticity, namely structural HOMA (harmonic oscillator model of aromaticity) and magnetic NICS (nucleus independent chemical shift) aromaticity indices, in particular, the NICS$_{zz}(+1)$ component. Finally, possible numerical checks on the conditions relating to validity of the well-known Yamaguchi’s formula for calculating the exchange coupling coefficient J in diradical systems are discussed.
Toward sustainable fuel cells

A quarter of humanity's current energy consumption is used for transportation (1). Low-temperature hydrogen fuel cells offer much promise for replacing this colossal use of fossil fuels with renewables; these fuel cells produce negligible emissions and have a mileage and filling time equal to a regular gasoline car. However, current fuel cells require 0.25 g of platinum (Pt) per kilowatt of power (2) as catalysts to drive the electrode reactions. If the entire global annual production of Pt were devoted to fuel cell vehicles, fewer than 10 million vehicles could be produced each year, a mere 10% of the annual automotive vehicle production. Lowering the Pt loading in a fuel cell to a sustainable level requires the reactivity of Pt to be tuned so that it accelerates oxygen reduction more effectively (3). Two reports in this issue address this challenge (4, 5).
Main Research Area: Technical/natural sciences

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BFI (2014): BFI-level 2
Scopus rating (2014): SJR 12.052 SNIP 8.129 CiteScore 12.68
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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
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Tunable waveguide and cavity in a phononic crystal plate by controlling whispering-gallery modes in hollow pillars

We investigate the properties of a phononic crystal plate with hollow pillars and introduce the existence of whispering-gallery modes (WGMs). We show that by tuning the inner radius of the hollow pillar, these modes can merge inside both Bragg and low frequency band gaps, deserving phononic crystal and acoustic metamaterial applications. These modes can be used as narrow pass bands for which the quality factor can be greatly enhanced by the introduction of an additional cylinder between the hollow cylinder and the plate. We discuss some functionalities of these confined WGM in both Bragg and low frequency gaps for wavelength division in multiplexer devices using heteroradii pillars introduced into waveguide and cavity structures.

**General information**

State: Published

Organisations: Department of Physics, Centre National de la Recherche Scientifique, Institut des Nanosciences de Paris, Tongji University

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- Web of Science (2017): Indexed yes
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- Web of Science (2016): Indexed yes
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- Web of Science (2014): Indexed yes
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- Scopus rating (2012): SJR 3.173 SNIP 1.378 CiteScore 3.57
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- Web of Science (2012): Indexed yes
- Scopus rating (2011): SJR 3.262 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
Tuning Conductance in Aromatic Molecules: Constructive and Counteractive Substituent Effects

Destructive quantum interference in aromatic hydrocarbons can be tuned using chemical substituents; however, classical chemical intuition is not enough to explain the effects on electron transport. Using Hückel theory and density functional theory calculations, in combination with the Landauer-Buttiker approach for charge transport, novel substituent effects are demonstrated. For a 1,3-linked benzene, an electron acceptor in position 2 is shown to have the same effect on the antiresonance energy as an electron donor in position 4 and vice versa. Substituents in position 5 have no effect on the antiresonance energy. The effects appear to be additive, such that a donor in position 2 will counteract a donor in position 4, leading to cancellation of the substituent effect. Counter- and nonactive substituent positions exist for all aromatic hydrocarbons and can be predicted using a diagrammatic approach. This insight should be useful when substituents are to be used for tuning destructive quantum interference features in the transmission relative to the Fermi energy of the electrodes.
In this paper we discuss how different feedback gratings affect the tuning range and the output power of external feedback diode laser systems. A tunable high-power narrow-spectrum external-cavity diode laser system around 455 nm is investigated. The laser system is based on a high-power GaN diode laser in a Littrow external-cavity. Both a holographic diffraction grating and a ruled diffraction grating are used as feedback elements in the external cavity. The output power,
spectral bandwidth, and tunable range of the external cavity diode laser system are measured and compared with the two gratings at different injected currents. When the holographic grating is used, the laser system can be tuned over a range of 1.4 nm with an output power around 530 mW. When the ruled grating is used, the laser system can be tuned over a range of 6.0 nm with an output power around 80 mW. The results can be used as a guide for selecting gratings for external-cavity diode lasers for different requirements. (C) 2016 Optical Society of America
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 (Pt)–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.
Tunneling spectra of graphene on copper unraveled

Scanning tunneling spectroscopy is often employed to study two-dimensional (2D) materials on conductive growth substrates, in order to gain information on the electronic structures of the 2D material-substrate systems, which can lead to insight into 2D material-substrate interactions, growth mechanisms, etc. The interpretation of the spectra can be complicated, however. Specifically for graphene grown on copper, there have been conflicting reports of tunneling spectra. A clear understanding of the mechanisms behind the variability is desired. In this work, we have revealed that the root cause of the variability in tunneling spectra is the variation in graphene-substrate coupling under various experimental conditions, providing a salutary perspective on the important role of 2D material-substrate interactions. The conclusions are drawn from measured data and theoretical calculations for monolayer, AB-stacked bilayer, and twisted bilayer graphene coexisting on the same substrates in areas with and without intercalated oxygen, demonstrating a high degree of consistency. The Van Hove singularities of the twisted graphene unambiguously indicate the Dirac energy between them, lending strong evidence to our assignment of the spectral features. In addition, we have discovered an O-Cu superstructure that has never been observed before.

General information
State: Published
Organisations: Department of Micro- and Nanotechnology, Theoretical Nanoelectronics, Department of Physics, Center for Nanostructured Graphene, University at Buffalo, University of Tennessee
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Scopus rating (2016): CiteScore 4.06 SJR 1.685 SNIP 1.113
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BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.725 SNIP 1.205 CiteScore 4.45
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BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.771 SNIP 1.239 CiteScore 4.29
Web of Science (2014): Indexed yes
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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
Two-phase model of hydrogen transport to optimize nanoparticle catalyst loading for hydrogen evolution reaction

With electrocatalysts it is important to be able to distinguish between the effects of mass transport and reaction kinetics on the performance of the catalyst. When the hydrogen evolution reaction (HER) is considered, an additional and often neglected detail of mass transport in liquid is the evolution and transport of gaseous H2, since HER leads to the continuous formation of H2 bubbles near the electrode. We present a numerical model that includes the transport of both gaseous and dissolved H2, as well as mass exchange between them, and combine it with a kinetic model of HER at platinum (Pt) nanoparticle electrodes.

We study the effect of the diffusion layer thickness and H2 dissolution rate constant on the importance of gaseous transport, and the effect of equilibrium hydrogen coverage and Pt loading on the kinetic and mass transport overpotentials. Gaseous transport becomes significant when the gas volume fraction is sufficiently high to facilitate H2 transfer to bubbles within a distance shorter than the diffusion layer thickness. At current densities below about 40 mA/cm2 the model reduces to an analytical approximation that has characteristics similar to the diffusion of H2. At higher current densities the increase in the gas volume fraction makes the H2 surface concentration nonlinear with respect to the current density. Compared to the typical diffusion layer model, our model is an extension that allows more detailed studies of reaction kinetics and mass transport in the electrolyte and the effects of gas bubbles on them.

General information
State: Published
Organisations: Department of Micro- and Nanotechnology, Silicon Microtechnology, Department of Physics, Experimental Surface and Nanomaterials Physics, Aalto University
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BFI (2016): BFI-level 2
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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
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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
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Ultrafast Excited State Relaxation of a Metalloporphyrin Revealed by Femtosecond X-ray Absorption Spectroscopy

Photoexcited Nickel(II) tetramesitylporphyrin (NiTMP), like many open-shell metalloporphyrins, relaxes rapidly through multiple electronic states following an initial porphyrin-based excitation, some involving metal centered electronic configuration changes that could be harnessed catalytically before excited state relaxation. While a NiTMP excited state present at 100 ps was previously identified by X-ray transient absorption (XTA) spectroscopy at a synchrotron source as a relaxed (d,d) state, the lowest energy excited state (J. Am. Chem. Soc., 2007, 129, 9816 and Chem. Sci., 2010, 1, 642), structural dynamics before thermalization were not resolved due to the similar to 100 ps duration of the available X-ray probe pulse. Using the femtosecond (fs) X-ray pulses of the Linac Coherent Light Source (LCLS), the Ni center electronic configuration from the initial excited state to the relaxed (d,d) state has been obtained via ultrafast Ni K-edge XANES (X-ray absorption near edge structure) on a time scale from hundreds of femtoseconds to 100 ps. This enabled the identification of a short-lived Ni(I) species aided by time-dependent density functional theory (TDDFT) methods. Computed electronic and nuclear structure for critical excited electronic states in the relaxation pathway characterize the dependence of the complex's geometry on the electron occupation of the 3d orbitals. Calculated XANES transitions for these excited states assign a short-lived transient signal to the spectroscopic signature of the Ni(I) species, resulting from intramolecular charge transfer on a time scale that has eluded previous synchrotron studies. These combined results enable us to examine the excited state structural dynamics of NiTMP prior to thermal relaxation and to capture intermediates of potential photocatalytic significance.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, SLAC National Accelerator Laboratory, Argonne National Laboratory, University of Washington, Northwestern University
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Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 13.18 SJR 7.492 SNIP 2.596
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 6.775 SNIP 2.63 CiteScore 12.81
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 6.294 SNIP 2.587 CiteScore 11.92
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 5.993 SNIP 2.466 CiteScore 11.38
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Uncertainty budget for determinations of mean isomer shift from Mössbauer spectra

The magnetite/maghemite content within iron oxide nanoparticles can be determined using the mean isomer shift ($\delta_{\text{mean}}$). However, accurate characterisation of the composition is limited by the uncertainty associated with $\delta_{\text{mean}}$. We have identified four independent sources of uncertainty and developed a quantitative expression for the uncertainty budget. Sources of uncertainty are categorised as follows: that from the fitting of the Mössbauer spectrum ($\sigma_{\text{fit}}$), that of the calibration of the $\alpha$-Fe reference spectrum ($\sigma_{\text{cal}}$), thermal corrections to the spectrum due to second order Doppler shift (SODS) ($\sigma_{\Delta\delta}$) and other experimental errors ($\sigma_{\text{err}}$). Each contribution is discussed in detail using $^{57}$Fe Mössbauer spectra obtained from an iron oxide nanoparticle system at temperatures between 16 K and 295 K on different spectrometers in two different laboratories.

General information
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Organisations: Department of Micro- and Nanotechnology, Magnetic Systems, Department of Physics, Neutrons and X-rays for Materials Physics, Physikalisch-Technische Bundesanstalt, University College London
Universal amorphous-amorphous transition in Ge$_x$Se$_{100-x}$ glasses under pressure

Pressure induced structural modifications in vitreous Ge$_x$Se$_{100-x}$ (where 10 ≤ x ≤ 25) are investigated using X-ray absorption spectroscopy (XAS) along with supplementary X-ray diffraction (XRD) experiments and ab initio molecular dynamics (AIMD) simulations. Universal changes in distances and angle distributions are observed when scaled to reduced densities. All compositions are observed to remain amorphous under pressure values up to 42 GPa. The Ge-Se interatomic distances extracted from XAS data show a two-step response to the applied pressure; a gradual decrease followed by an increase at around 15–20 GPa, depending on the composition. This increase is attributed to the metallization event that can be traced with the red shift in Ge K edge energy which is also identified by the principal peak position of the structure factor. The densification mechanisms are studied in details by means of AIMD simulations and compared to the experimental results. The evolution of bond angle distributions, interatomic distances and coordination numbers are examined and lead to similar pressure-induced structural changes for any composition.
University Campus and Collections Combining as A Cultural Landscape – Nudging and Critical Thinking

Many university collections have special connections with places and institutions. Both the collections and the places speak volume about the institutions. They tell stories about values, traditions, history, practices, assumptions and myths connected to an institution for those who tune in. In this paper we will discuss how combining the collections and the university campuses can be used to create contemplation and raise questions about the university itself amongst students. How can we use collections to create a cultural landscape at the university which increases ownership of own education? Can we make students recognize and contemplate unseen boundaries, practices and identities, which university life is installing into them? Can we turn campuses into giant teaching tools, which will confront and nudge the students as they use the spaces? The paper will also discuss how to approach university students as an audience. They have specialist knowledge in specific topics. Should we treat them as a unique audience type and can we use the activity, dialogue and participation tools, which are seen as important for constructing new knowledge in museums? Can we use the bodily experience of the place? Can we use social media, exhibits and other means to create a cultural landscape at university with more than three dimensions? Drawing on experiences from the work of the History of Technology division at DTU we will examine these questions.

General information
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Organisations: Department of Physics
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Upconversion-based lidar measurements of atmospheric CO2

For the first time an upconversion based detection scheme is demonstrated for lidar measurements of atmospheric CO2-concentrations, with a hard target at a range of 3 km and atmospheric backscatter from a range of similar to 450 m. The pulsed signals at 1572 nm are upconverted to 635 nm, and detected by a photomultiplier tube, to test how the upconversion technology performs in a long range detection system. The upconversion approach is compared to an existing direct detection scheme using a near-IR detector with respect to signal-to-noise ratio and quantum efficiency. It is for the first time analyzed how the field-of-view of a receiver system, for long range detection, depends critically on the parameters for the nonlinear upconversion process, and how to optimize these parameters in future systems. (C) 2016 Optical Society of America

General information
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Organisations: Department of Photonics Engineering, Optical Sensor Technology, Department of Physics, Risø National Laboratory for Sustainable Energy, DLR
Authors: Hegstedt, L. (Intern), Fix, A. (Ekstern), Wirth, M. (Ekstern), Pedersen, C. (Intern), Tidemand-Lichtenberg, P. (Intern)
Upconversion imaging using an all-fiber supercontinuum source

In this Letter, the first demonstration, to the best of our knowledge, of pulsed upconversion imaging using supercontinuum light is presented. A mid-infrared (IR) imaging system was built by combining a mid-IR supercontinuum source emitting between 1.8 and 2.6 μm with upconversion detection. The infrared signal is used to probe a sample and mixed with a synchronized 1550 nm laser pulse inside a lithium niobate (LiNbO3) crystal. The signal is thus upconverted to the 860-970 nm range and acquired on a standard silicon CCD array at a rate of 22 frames per second. In our implementation, spatial features in the sample plane as small as 55 μm could be resolved. (C) 2016 Optical Society of America

General information
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Organisations: Department of Photonics Engineering, Department of Physics, Optical Sensor Technology, Risø National Laboratory for Sustainable Energy, NKT Photonics A/S
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Web of Science (2015): Indexed yes
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Scopus rating (2014): SJR 2.429 SNIP 1.997 CiteScore 3.86
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Velocity-space tomography of fusion plasmas by collective Thomson scattering of gyrotron radiation

We propose a diagnostic capable of measuring 2D fast-ion velocity distribution functions \( f_2 \) in the MeV-range in magnetized fusion plasmas. Today velocity-space tomography based on fast-ion D\( ^{2} \) spectacle spectroscopy is regularly used to measure \( f_2 \) for ion energies below 100 keV. Unfortunately, the signal-to-noise ratio becomes fairly low for MeV-range ions. Ions at any energy can be detected well by collective Thomson scattering of mm-wave radiation from a high-power gyrotron. We demonstrate how collective Thomson scattering can be used to measure \( f_2 \) in the MeV-range in reactor relevant plasmas such as in the tokamaks ITER or DEMO.
Verification of BOUT++ plus plus by the method of manufactured solutions

BOUT++ is a software package designed for solving plasma fluid models. It has been used to simulate a wide range of plasma phenomena ranging from linear stability analysis to 3D plasma turbulence and is capable of simulating a wide range of drift-reduced plasma fluid and gyro-fluid models. A verification exercise has been performed as part of a EUROfusion Enabling Research project, to rigorously test the correctness of the algorithms implemented in BOUT++, by testing order-of-accuracy convergence rates using the Method of Manufactured Solutions (MMS). We present tests of individual components including time-integration and advection schemes, nonorthogonal toroidal field-aligned coordinate systems and the shifted metric procedure which is used to handle highly sheared grids. The flux coordinate independent approach to differencing along magnetic field-lines has been implemented in BOUT++ and is here verified using the MMS in a sheared slab configuration. Finally, we show tests of three complete models: 2-field Hasegawa-Wakatani in 2D slab, 3-field reduced magnetohydrodynamics (MHD) in 3D field-aligned toroidal coordinates, and 5-field reduced MHD in slab geometry.
Visualizing the mobility of silver during catalytic soot oxidation

The catalytic activity and mobility of silver nanoparticles used as catalysts in temperature programmed oxidation of soot:silver (1:5 wt:wt) mixtures have been investigated by means of flow reactor experiments and in situ environmental transmission electron microscopy (ETEM). The carbon oxidation temperature was significantly lower compared to uncatalyzed soot oxidation with soot and silver loosely stirred together (loose contact) and lowered further with the two components crushed together (tight contact). The in situ TEM investigations revealed that the silver particles exhibited significant mobility during the soot oxidation, and this mobility, which increases the soot/catalyst contact, is expected to be an important factor for the lower oxidation temperature. In the intimate tight contact mixture the initial dispersion of the silver particles is greater, and the onset of mobility occurs at a lower temperature which is consistent with the lower oxidation temperature of the tight contact mixture. (C) 2015 Elsevier B.V. All rights reserved.
Water at Interfaces

The interfaces of neat water and aqueous solutions play a prominent role in many technological processes and in the environment. Examples of aqueous interfaces are ultrathin water films that cover most hydrophilic surfaces under ambient relative humidities, the liquid/solid interface which drives many electrochemical reactions, and the liquid/vapor interface, which governs the uptake and release of trace gases by the oceans and cloud droplets. In this article we review some of the recent experimental and theoretical advances in our knowledge of the properties of aqueous interfaces and discuss open questions and gaps in our understanding.

General information
State: Published
Organisations: Department of Physics, Theoretical Atomic-scale Physics, Uppsala University, University of Liverpool, University College London, Princeton University, University of Copenhagen, KTH - Royal Institute of Technology, Lawrence Berkeley National Laboratory, Peking University
Authors: Björneholm, O. (Ekstern), Hansen, M. H. (Intern), Hodgson, A. (Ekstern), Liu, L. (Ekstern), Limmer, D. T. (Ekstern), Michaelides, A. (Ekstern), Pedevilla, P. (Ekstern), Rossmeisl, J. (Ekstern), Shen, H. (Ekstern), Tocci, G. (Ekstern), Tyrode, E. (Ekstern), Walz, M. (Ekstern), Werner, J. (Ekstern), Bluhm, H. (Ekstern)
Number of pages: 29
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Main Research Area: Technical/natural sciences

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Web of Science (2017): Indexed yes
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Scopus rating (2015): SJR 18.035 SNIP 11.285 CiteScore 45.92
Web of Science (2015): Indexed yes
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Scopus rating (2014): SJR 18.38 SNIP 11.392 CiteScore 44.56
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 22.299 SNIP 12.788 CiteScore 49.12
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 2
Water-Mediated Ion Pairing: Occurrence and Relevance

We present an overview of the studies of ion pairing in aqueous media of the past decade. In these studies, interactions between ions, and between ions and water, are investigated with relatively novel approaches, including dielectric relaxation spectroscopy, far-infrared (terahertz) absorption spectroscopy, femtosecond mid-infrared spectroscopy, and X-ray spectroscopy and scattering, as well as molecular dynamics simulation methods. With these methods, it is found that ion pairing is not a rare phenomenon only occurring for very particular, strongly interacting cations and anions. Instead, for many salt solutions and their interfaces, the measured and calculated structure and dynamics reveal the presence of a distinct concentration of contact ion pairs (CIPs), solvent shared ion pairs (SIPs), and solvent-separated ion pairs (2SIPs).

We discuss the importance of specific ion-pairing interactions between cations like Li(+) and Na(+) and anionic carboxylate and phosphate groups for the structure and functioning of large (bio)molecular systems.

General information

State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Technische Universität Darmstadt, Ecole Polytechnique Federale de Lausanne (EPFL), Lund University, FOM Institute for Atomic and Molecular Physics - AMOLF, Peking University
Authors: van der Vegt, N. F. (Ekstern), Haldrup, K. (Intern), Roke, S. (Ekstern), Zheng, J. (Ekstern), Lund, M. (Ekstern), Bakker, H. J. (Ekstern)
Number of pages: 16
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Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information

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The work of this thesis revolves around catalytic activity measurements of nano-particles tested using a μ-reactor platform, developed and produced at DTU, in a collaboration between CINF and Nanotech. The thesis contains the results from two separate research projects; both utilising μ-reactors in combination with surface...
science techniques and computer simulations. The first project described is a study of hydrogen dissociation on monodisperse platinum clusters. The second project studies methanation from carbon monoxide and hydrogen on nanoparticles of nickel-iron alloys. The second study is a work in progress, and the corresponding chapter aims to summarise the results so far. Other projects are not included in the thesis because they are inconclusive or dead ends. Hydrogen dissociation was studied by the $\text{H}_2/\text{D}_2$ exchange reaction on SiO$_2$-supported mono-disperse platinum clusters in a reactor. The reaction was tested under ambient pressures and temperatures ranging from room temperature to 180 °C. The initial ambition was to study size effects on the chemical activity of clusters, but experimental challenges prevented a final conclusion on cluster size effects. Using Pt$_8$ cluster samples it was found that minute amounts of oxygen present in the gas stream would change the clusters ability to dissociate hydrogen. Reaction products were analysed with quadrupole mass spectrometry. The catalyst was characterized before and after chemical testing using XPS and ISS, proving the catalyst to be highly stable. DFT simulations demonstrated that even a single oxygen atom binds strongly to SiO$_2$-supported Pt$_8$ clusters and changes the morphology and chemical properties of the cluster.

Catalytic methanation reaction from CO and H$_2$ was studied on Ni$_{75}$Fe$_{25}$ nano-particles with sizes 3.5nm, 5nm, 7nm and 9nm. The presented data is a work in progress, but initial results show a tendency of 7nm particles being most active. The catalyst is characterized before and after chemical activity measurements using ISS, XPS, and SEM to ensure a clean surface and consistent deposition. Plans for the immediate future involve reproducing activity measurements on all sample sizes and more consistent characterisation with ISS and XPS. An ambitious plan is to do a similar size study on pure nickel nano-particles, to examine differences and similarities between the catalysts under reaction conditions.

**General information**

State: Published
Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics
Authors: Riedel, J. N. (Intern), Chorkendorff, I. (Intern)
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Main Research Area: Technical/natural sciences
Electronic versions: PhD_thesis_Riedel_.pdf

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Projects:

μ-reactor measurements of catalytic activity of mass selected nano-particles
Publication: Research › Ph.D. thesis – Annual report year: 2016

**Catalysts for selective oxidation of ammonia in a gas containing hydrogen.**
The invention contributes to a cost effective way to solve the problem of trace ammonia removal from a hydrogen and nitrogen containing gas. The set of catalysts of the invention selectively oxidised ammonia in ppm concentration even in gas mixtures containing hydrogen gas in concentrations of three orders of magnitude higher than the concentration of ammonia.

**General information**

State: Published
Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics
Authors: Chorkendorff, I. (Intern), Chakraborty, D. (Intern), Olsen, J. L. (Intern), Silva, H. J. L. (Intern), Nielsen, M. G. (Intern)
Publication date: 3 Dec 2015

**Publication information**

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Priority number: EP201406994
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Main Research Area: Technical/natural sciences
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)
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Catalyst for Ammonia Oxidation
The present invention relates to a bimetallic catalyst for ammonia oxidation, a method for producing a bimetallic catalyst for ammonia oxidation and a method for tuning the catalytic activity of a transition metal. By depositing an overlayer of less catalytic active metal onto a more catalytic active metal, the total catalytic activity is enhanced.

General information
State: Published
Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics
Authors: Conradsen, C. N. (Intern), Olesen, S. E. (Intern), Chakraborty, D. (Intern), Chorkendorff, I. (Intern)
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Publication information
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Priority number: EP20130196039
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Also registered as: WO2014EP73293, EP20130196039
Main Research Area: Technical/natural sciences
Source: espacenet
Source-ID: WO2015082141
Publication: Research › Patent – Annual report year: 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)
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Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, European Spallation Source ESS AB, Business Region Skåne, University of California at Berkeley, J-PARC, Lund University
Authors: Cereser, A. (Intern), Strobl, M. (Ekstern), Hall, S. (Ekstern), Steuwer, A. (Ekstern), Tremsin, A. (Ekstern), Bergbäck Knudsen, E. (Intern), Willendrup, P. K. (Intern), Kiyanagi, R. (Ekstern), Shinohara, T. (Ekstern), Schmidt, S. (Intern)
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Authors: Cereser, A. (Intern), Strobl, M. (Ekstern), Hall, S. (Ekstern), Steuwer, A. (Ekstern), Tremsin, A. (Ekstern), Bergbäck Knudsen, E. (Intern), Willendrup, P. K. (Intern), Kockelmann, W. (Ekstern), Peeertmans, S. (Ekstern), Shinohara, T. (Ekstern), Schmidt, S. (Intern)
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Event: Poster session presented at 4th Annual Niels Bohr International Academy Workshop-School on ESS Science, Copenhagen, Denmark.
Main Research Area: Technical/natural sciences
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3D particle tracking velocimetry using dynamic discrete tomography
Particle tracking velocimetry in 3D is becoming an increasingly important imaging tool in the study of fluid dynamics and combustion as well as plasmas. We introduce a dynamic discrete tomography algorithm for reconstructing particle trajectories from projections. The algorithm is efficient for data from two projection directions and exact in the sense that it finds a solution consistent with the experimental data. Non-uniqueness of solutions can be detected and solutions can be tracked individually.

General information
State: Published
Organisations: Department of Physics, Plasma Physics and Fusion Energy, Technische Universität München, FOM Dutch Institute for Fundamental Energy Research
Authors: Alpers, A. (Ekstern), Gritzmann, P. (Ekstern), Moseev, D. (Ekstern), Salewski, M. (Intern)
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Scopus rating (2016): CiteScore 4.04 SJR 1.914 SNIP 2.094
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Scopus rating (2014): SJR 1.344 SNIP 1.649 CiteScore 2.86
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Scopus rating (2013): SJR 1.455 SNIP 1.692 CiteScore 3.17
ISI indexed (2013): ISI indexed yes
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Scopus rating (2012): SJR 2.11 SNIP 2.162 CiteScore 3.46
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Scopus rating (2011): SJR 1.75 SNIP 1.951 CiteScore 3.22
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
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Web of Science (2010): Indexed yes
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Scopus rating (2009): SJR 1.228 SNIP 1.266
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.228 SNIP 1.172
Ab initio quantum-enhanced optical phase estimation using real-time feedback control

Optical phase estimation is a vital measurement strategy that is used to perform accurate measurements of various physical quantities including length, velocity and displacements(1,2). The precision of such measurements can be greatly enhanced by the use of entangled or squeezed states of light as demonstrated in a variety of different optical systems(3-8). Most of these accounts, however, deal with the measurement of a very small shift of an already known phase, which is in stark contrast to ab initio phase estimation where the initial phase is unknown(9-12). Here, we report on the realization of a quantum-enhanced and fully deterministic ab initio phase estimation protocol based on real-time feedback control. Using robust squeezed states of light combined with a real-time Bayesian adaptive estimation algorithm, we demonstrate deterministic phase estimation with a precision beyond the quantum shot noise limit. The demonstrated protocol opens up new opportunities for quantum microscopy, quantum metrology and quantum information processing.

General information
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Organisations: Department of Physics, Quantum Physics and Information Technology, Leibniz Universität Hannover, Università degli Studi di Milano
Authors: Berni, A. (Intern), Gehring, T. (Intern), Nielsen, B. M. (Intern), Händchen, V. (Ekstern), Paris, M. G. A. (Ekstern), Andersen, U. L. (Intern)
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BFI (2015): BFI-level 2
Web of Science (2015): Indexed yes
Ab Initio Thermodynamic Modeling of Electrified Metal-Oxide Interfaces: Consistent Treatment of Electronic and Ionic Chemical Potentials

Solid oxide fuel cells are attractive devices in a sustainable energy context because of their fuel flexibility and potentially highly efficient conversion of chemical to electrical energy. The performance of the device is to a large extent determined by the atomic structure of the electrode-electrolyte interface. Lack of atomic-level information about the interface has limited the fundamental understanding, which further limits the opportunity for optimization. The atomic structure of the interface is affected by electrode potential, chemical potential of oxygen ions, temperature and gas pressures. Here we present a scheme to determine the metal-oxide interface structure at a given set of these environmental parameters based on quantum chemical calculations. As an illustration we determine the structure of a Ni-YSZ anode as a function of electrode potential at 0 and 1000 K. We further describe how the structural information can be used as a starting point for accurate calculations of the kinetics of fuel oxidation reactions, in particular the hydrogen oxidation reaction. More generally, we anticipate that the scheme will be a valuable theoretical tool to describe solid-solid interfaces. [Figure]
Acetaldehyde as an intermediate in the electroreduction of carbon monoxide to ethanol on oxide-derived copper

General information
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Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics, Department of Chemistry, Organic Chemistry, Carlsberg Laboratory
Number of pages: 1
Publication date: 2015

Acoustic streaming in microchannels: The trinity of analytics, numerics and experiments
This thesis presents studies of boundary-driven acoustic streaming in microfluidic channels, which is a steady flow of the fluid initiated by the interactions of an oscillating acoustic standing wave and the rigid walls of the microchannel. The studies present analysis of the acoustic resonance, the acoustic streaming flow, and the forces on suspended microparticles. The work is motivated by the application of particle focusing by acoustic radiation forces in medical, environmental and food sciences. Here acoustic streaming is most often unwanted, because it limits the focusability of particles smaller than a given critical size. One of the main goals of this thesis work has been to overcome this limitation. The main text of this thesis serves to give an introduction to the theory and numerical models applied in the five journal papers supplied in the Appendixes, which constitute this thesis work.

Based on first- and second-order perturbation theory, assuming small acoustic amplitudes, we derived the time-dependent governing equations under adiabatic conditions. The adiabatic first- and second-order equations are solved analytically for the acoustic field between two orthogonally oscillating plates. Furthermore, under general thermodynamic conditions, we derive the time-dependent first- and second-order equations for the conservation of mass, momentum, and energy. The coupling from fluid equations to particle motion is achieved through the expressions for the streaming-induced drag force and the acoustic radiation force acting on particles suspended in the fluid. Lastly, the numerical method is discussed, with emphasis on how proper numerical convergence is ensured.

Three numerical studies are presented, in which the acoustic resonance and the acoustic streaming flow are investigated, both in the transient regime and in the purely periodic state. The solutions for the periodic acoustic resonance and the steady streaming flow are used to simulate the motion of suspended particle in a Lagrangian description, which mimics experimental particle tracking velocimetry.

In the forth study, the numerical model is used to engineer a single roll streaming flow, which does not counteract the focusing by the acoustic radiation force, contrary to the usual quadrupolar streaming flow. The single roll streaming flow is observed experimentally in a nearly-square channel, and acoustophoretic focusing of E. coli bacteria and 0.6 µm particles is achieved. These particles are considerably smaller than the critical particle size of approximately 2 µm for the usual half-wavelength resonance in a rectangular channel.

The fifth study presents a quantitative comparison of analytical, numerical, and experimental results for the streaming-induced drag force dominated motion of particles suspended in a water-filled microchannel supporting a transverse half-wavelength resonance. The experimental and theoretical results agree within a mean relative dierence of approximately 20%, a low deviation given state-of-the-art in the field. Furthermore, the analytical solution for the acoustic streaming in rectangular channels with arbitrary large height-to-width ratios is derived. This accommodates the analytical theory of acoustic streaming to applications within acoustofluidics.

General information
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Active Site Engineering in Electrocatalysis

The overall goal of this thesis has been to design better catalysts for electrochemical reactions through a fundamental understanding of the materials at atomic scale. This has been achieved by combining electrochemical measurements with a variety of characterization techniques, often in ultra high vacuum, as well as theory calculations. The thesis falls in three different parts: firstly, study of model systems for oxygen reduction to water; secondly, oxygen reduction to hydrogen peroxide on both model systems and commercially relevant nanoparticles and thirdly CO2 and CO electroreduction studies on nanostructured electrodes.

• Oxygen reduction to water has been carried out on Pt-rare earth alloys, which outperformed the activity of Pt by as much as a factor of five while showing promising stability. The increase in activity can be attributed to compressive strain of the Pt overlayer formed under reaction conditions, which is ultimately controlled by the crystal structure of the underlying alloy.

• Oxygen reduction to hydrogen peroxide has been investigated on single site catalysts, mainly alloys of noble metals with Hg. This resulted in a very special structure with isolated atoms of Pt or Pd surrounded by Hg, which greatly enhanced selectivity to H2O2 during oxygen reduction. Compared to state-of-the-art Au-based catalysts, Pt-Hg and Pd-Hg alloys present over 20 and 100 times increase in mass activity respectively. It was proven that activity for this reaction is controlled by the binding energy of the sole reaction intermediate.

• CO2 and CO electroreduction studies have attempted to understand the unprecedented activity of oxide-derived Cu recently reported in the literature. Temperature programmed desorption measurements reveal very strong CO binding at these surfaces, inexisten in other forms of Cu. The presence of strong CO binding sites correlates well with electrochemical activity, which paves the way for the rational development of even better electrocatalysts.

General information

State: Published
Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics
Authors: Verdaguer Casadevall, A. (Intern), Stephens, I. (Intern), Chorkendorff, I. (Intern)
Number of pages: 146
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A design study of VOR: A versatile optimal resolution chopper spectrometer for the ESS

VOR, the versatile optimal resolution chopper spectrometer, is designed to probe dynamic phenomena that are currently inaccessible for inelastic neutron scattering due to flux limitations. VOR is a short instrument by the standards of the European Spallation Source (ESS), 30.2m moderator to sample, and provides instantaneous access to a broad dynamic range, 1-120 meV within each ESS period. The short instrument length combined with the long ESS pulse width enables a quadratic flux increase, even at longer wavelengths, by relaxing energy resolution from ΔE/E = 1% up to ΔE/E = 7%. This is impossible both on a long chopper spectrometer at the ESS and with instruments at short pulsed sources. In comparison to current day chopper spectrometers, VOR can offer an order of magnitude improvement in flux for equivalent energy resolutions, ΔE/E = 1-3%. Further relaxing the energy resolution enables VOR to gain an extra order of magnitude in flux. In addition, VOR has been optimised for repetition rate multiplication (RRM) and is therefore able to measure, in a single ESS period, 6-14 incident wavelengths, across a wavelength band of 9 Å with a novel chopper configuration that transmits all incident wavelengths with equivalent counting statistics. The characteristics of VOR make it a unique instrument with capabilities to access small, limited-lifetime samples and transient phenomena with inelastic neutron scattering.
We present calculations of the correlation energies of crystalline solids and isolated systems within the adiabatic-connection fluctuation-dissipation formulation of density-functional theory. We perform a quantitative comparison of a set of model exchange-correlation kernels originally derived for the homogeneous electron gas (HEG), including the recently introduced renormalized adiabatic local-density approximation (rALDA) and also kernels which (a) satisfy known exact limits of the HEG, (b) carry a frequency dependence, or (c) display a 1/k² divergence for small wavevectors. After generalizing the kernels to inhomogeneous systems through a reciprocal-space averaging procedure, we calculate the lattice constants and bulk moduli of a test set of 10 solids consisting of tetrahedrally bonded semiconductors (C, Si, SiC), ionic compounds (MgO, LiCl, LiF), and metals (Al, Na, Cu, Pd). We also consider the atomization energy of the H₂ molecule. We compare the results calculated with different kernels to those obtained from the random-phase approximation (RPA) and to experimental measurements. We demonstrate that the model kernels correct the RPA's tendency to overestimate the magnitude of the correlation energy whilst maintaining a high-accuracy description of structural properties.
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Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.13 SJR 1.486 SNIP 0.964
Web of Science (2016): Indexed yes
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Scopus rating (2015): SJR 1.255 SNIP 0.964 CiteScore 1.98
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.446 SNIP 1.02 CiteScore 2.54
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.559 SNIP 1.174 CiteScore 2.95
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.832 SNIP 1.137 CiteScore 2.86
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.845 SNIP 1.215 CiteScore 3.07
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.777 SNIP 1.064
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.04 SNIP 1.119
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 2.27 SNIP 1.144
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 2.245 SNIP 1.13
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 2.254 SNIP 1.287
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 2.323 SNIP 1.349
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 2.272 SNIP 1.39
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 2.275 SNIP 1.395
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 2.28 SNIP 1.382
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 2.549 SNIP 1.375
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 1.947 SNIP 1.441
Advancing Fusion by Innovations: Smaller, Quicker, Cheaper: Paper

On the path to Fusion power, the construction of ITER is on-going, however there is not much progress in performance improvements of tokamaks in the last 15 years, Fig.1. One possible reason for this stagnation is the lack of innovations in physics and technology that could be implemented with this approach in which progress is expected mainly from the increase in the size of a Fusion device. Such innovations could be easier to test and use in much smaller (and so cheaper and quicker to build) compact Fusion devices. In this paper we propose a new path to Fusion energy based on a compact high field Spherical Tokamak approach.
A Heteroleptic Ferrous Complex with Mesoionic Bis(1,2,3-triazol-5-ylidene) Ligands: Taming the MLCT Excited State of Iron(II)

Strongly sigma-donating N-heterocyclic carbenes (NHCs) have revived research interest in the catalytic chemistry of iron, and are now also starting to bring the photochemistry and photophysics of this abundant element into a new era. In this work, a heteroleptic Fe-II complex (1) was synthesized based on sequentially furnishing the Fe-II center with the benchmark 2,2-bipyridine (bpy) ligand and the more strongly sigma-donating mesoionic ligand, 4,4-bis(1,2,3-triazol-5-ylidene) (btz). Complex 1 was comprehensively characterized by electrochemistry, static and ultrafast spectroscopy, and quantum chemical calculations and compared to [Fe(bpy)(3)](PF6)(2) and (TBA)(2)[Fe(bpy)(CN)(4)]. Heteroleptic complex 1 extends the absorption spectrum towards longer wavelengths compared to a previously synthesized homoleptic Fe-II NHC complex. The combination of the mesoionic nature of btz and the heteroleptic structure effectively destabilizes the metal-centered (MC) states relative to the triplet metal-to-ligand charge transfer ((MLCT)-M-3) state in 1, rendering it a lifetime of 13ps, the longest to date of a photochemically stable Fe-II complex. Deactivation of the (MLCT)-M-3 state is proposed to proceed via the (MC)-M-3 state that strongly couples with the singlet ground state.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Lund University, Uppsala University
Authors: Liu, Y. (Ekstern), Kjær, K. S. (Intern), Fredin, L. A. (Ekstern), Chabera, P. (Ekstern), Harlang, T. C. B. (Ekstern), Canton, S. E. (Ekstern), Lidin, S. (Ekstern), Zhang, J. (Ekstern), Lomoth, R. (Ekstern), Bergquist, K. (Ekstern), Persson, P. (Ekstern), Wärnmark, K. (Ekstern), Sundström, V. (Ekstern)
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): SNIP 1.02 SJR 2.265 CiteScore 4.9
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 5.03 SJR 2.352 SNIP 1.068
A Higgs at 125.1 GeV and baryon mass spectra derived from a Common U(3) Lie group framework

Baryons are described by a Hamiltonian on an intrinsic U(3) Lie group configuration space with electroweak degrees of freedom originating in specific Bloch wave factors. By opening the Bloch degrees of freedom pairwise via a U(2) Higgs mechanism, the strong and electroweak energy scales become related to yield the Higgs mass 125.085+/-0.017 GeV and
the usual gauge boson masses. From the same Hamiltonian we derive both the relative neutron to proton mass ratio and
the N and Delta mass spectra. All compare rather well with the experimental values. We predict neutral flavour baryon
singlets to be sought for in negative pions scattering on protons or in photoproduction on neutrons and in invariant mass
like \( \Sigma_c^+(2455)D^- \) from various decays above the opencharm threshold, e.g. at 4499, 4652 and 4723 MeV. The
fundamental predictions are based on just one length scale and the fine structure coupling. The interpretation is to
consider baryons as entire entities kinematically excited from laboratory space by three impact momentum generators,
three rotation generators and three Runge-Lenz generators to internalize as nine degrees of freedom covering colour, spin
and flavour. Quark and gluon fields come about when the intrinsic structure is projected back into laboratory space
depending on which exterior derivative one is taking. With such derivatives on the measurescaled wavefunction, we
derived approximate parton distribution functions for the u and d valence quarks of the proton that compare well with
established experimental analysis.

General information
State: Published
Organisations: Department of Physics, Department of Chemistry
Authors: Trinhammer, O. (Intern), Bohr, H. (Intern), Jensen, M. O. S. (Intern)
Number of pages: 8
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Journal: PoS - Proceedings of Science
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Ratings:
Scopus rating (2017): SJR 0.115 SNIP 0.023 CiteScore 0.05
Scopus rating (2016): SNIP 0.041 SJR 0.117
Scopus rating (2015): SNIP 0.035 SJR 0.119
Scopus rating (2014): SNIP 0.03 SJR 0.117
Scopus rating (2013): SNIP 0.022 SJR 0.116
ISI indexed (2013): ISI indexed no
Scopus rating (2012): SNIP 0.019 SJR 0.111
ISI indexed (2012): ISI indexed no
Scopus rating (2011): SNIP 0.009 SJR 0.107
ISI indexed (2011): ISI indexed no
Scopus rating (2010): SNIP 0.016 SJR 0.107
Scopus rating (2009): SNIP 0.012 SJR 0.105
Scopus rating (2008): SNIP 0.006 SJR 0.102
Scopus rating (2007): SNIP 0.002 SJR 0.101
Original language: English
Electronic versions:
A_Higgs_at_125.1_GeV_and_baryon_mass_spectra-derived_from_a_Common_U_3_Lie_group_framework.pdf

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Algebraic and algorithmic frameworks for optimized quantum measurements
von Neumann projections are the main operations by which information can be extracted from the quantum to the classical
realm. They are, however, static processes that do not adapt to the states they measure. Advances in the field of adaptive
measurement have shown that this limitation can be overcome by “wrapping” the von Neumann projectors in a higher-
dimensional circuit which exploits the interplay between measurement outcomes and measurement settings.
Unfortunately, the design of adaptive measurement has often been ad hoc and setup specific. We shall here develop a
unified framework for designing optimized measurements. Our approach is twofold: The first is algebraic and formulates
the problem of measurement as a simple matrix diagonalization problem. The second is algorithmic and models the
optimal interaction between measurement outcomes and measurement settings as a cascaded network of conditional
probabilities. Finally, we demonstrate that several figures of merit, such as Bell factors, can be improved by optimized
measurements. This leads us to the promising observation that measurement detectors which - taken individually - have a
low quantum efficiency can be arranged into circuits where, collectively, the limitations of inefficiency are compensated for.

**General information**
State: Published
Organisations: Department of Physics, Quantum Physics and Information Technology
Authors: Laghaout, A. (Intern), Andersen, U. L. (Intern)
Number of pages: 14
Publication date: 2015
Main Research Area: Technical/natural sciences

**Publication information**
Journal: Physical Review A
Volume: 92
Issue number: 4
ISSN (Print): 2469-9926
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 0.886 SJR 1.288 CiteScore 2.46
Web of Science (2017): Indexed yes
Scopus rating (2016): CiteScore 2.25 SJR 1.482 SNIP 0.985
Web of Science (2016): Indexed yes
Scopus rating (2015): SJR 1.747 SNIP 1.008 CiteScore 2.06
Web of Science (2015): Indexed yes
Scopus rating (2014): SJR 2.201 SNIP 1.163 CiteScore 2.46
Web of Science (2014): Indexed yes
Scopus rating (2013): SJR 2.305 SNIP 1.166 CiteScore 2.86
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Scopus rating (2012): SJR 2.519 SNIP 1.231 CiteScore 2.81
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
Scopus rating (2011): SJR 2.316 SNIP 1.252 CiteScore 2.79
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
Scopus rating (2010): SJR 2.4 SNIP 1.211
Web of Science (2010): Indexed yes
Scopus rating (2009): SJR 2.469 SNIP 1.346
Web of Science (2009): Indexed yes
Scopus rating (2008): SJR 2.536 SNIP 1.231
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 2.524 SNIP 1.203
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.834 SNIP 0.968
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.394 SNIP 0.806
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.473 SNIP 0.714
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.492 SNIP 0.925
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 2.066 SNIP 1.098
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 1.949 SNIP 1.356
A Linear Response DFT+U Study of Trends in the Oxygen Evolution Activity of Transition Metal Rutile Dioxides

There are known errors in oxidation energies of transition metal oxides caused by an improper treatment of their d-electrons. The Hubbard U is the computationally cheapest addition one can use to capture correct reaction energies, but the specific Hubbard U oftentimes must be empirically determined only when suitable experimental data exist. We evaluated the effect of adding a calculated, linear response U on the predicted adsorption energies, scaling relationships, and activity trends with respect to the oxygen evolution reaction for a set of transition metal dioxides. We find that applying a U greater than zero always causes adsorption energies to be more endothermic. Furthermore, the addition of the Hubbard U greater than zero does not break scaling relationships established without the Hubbard U. The addition of the calculated linear response U value produces shifts of different systems along the activity volcano that results in improved activity trends when compared with experimental results.

General information
State: Published
Organisations: Center for Atomic-scale Materials Design, Department of Physics, Carnegie Mellon University
Authors: Xu, Z. (Ekstern), Rossmeisl, J. (Intern), Kitchin, J. R. (Ekstern)
Number of pages: 7
Pages: 4827-4833
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: The Journal of Physical Chemistry Part C
Volume: 119
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): SJR 2.135 SNIP 1.147 CiteScore 4.58
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
All-silica microfluidic optical stretcher with acoustophoretic prefocusing

Acoustophoresis is a widely reported and used technique for microparticle manipulation and separation. In the study described here, acoustophoresis is employed to prefocus the flow (i.e., focusing occurring upstream of the analysis region) in a microfluidic chip intended for optical trapping and stretching. The whole microchip is made of silica with optical waveguides integrated by femtosecond laser writing. The acoustic force is produced by driving an external piezoelectric ceramic attached underneath the microchip at the chip resonance frequency. Thanks to an efficient excitation of acoustic waves in both water and glass, acoustophoretic focusing is observed along the channel length (>40 mm) and it is successfully demonstrated both with polystyrene beads, swollen red blood cell, and cells from mouse fibroblast cellular lines (L929).

General information
State: Published
Organisations: Department of Physics, Biophysics and Fluids, Università di Pavia, Politecnico di Milano
Authors: Nava, G. (Ekstern), Bragheri, F. (Ekstern), Yang, T. (Ekstern), Minzioni, P. (Ekstern), Osellame, R. (Ekstern), Cristiani, I. (Ekstern), Berg-Sørensen, K. (Intern)
Pages: 837-844
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Microfluidics and Nanofluidics
Volume: 19
Issue number: 4
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Analysis of deformation-induced intragranular orientation spread in IF-steel by a combination of 3DXRD and crystal plasticity

General information
State: Published
Organisations: Department of Mechanical Engineering, Materials and Surface Engineering, Department of Physics, Neutrons and X-rays for Materials Physics, European Synchrotron Radiation Facility
Authors: Winther, G. (Intern), Oddershede, J. (Intern), Wright, J. (Ekstern)
Number of pages: 1
Publication date: 2015
Event: Abstract from 17th International Conference on Textures of Materials, Dresden, Germany.
Main Research Area: Technical/natural sciences
Electronic versions:
3DXRD_crystal_plast.pdf
Analysis of the crystallographic and magnetic structures of the Tb$_{0.1}$Pr$_{0.9}$Al$_2$ and Tb$_{0.25}$Pr$_{0.75}$Al$_2$ magnetocaloric compounds by means of neutron scattering

Neutron powder diffraction and inelastic neutron scattering data were used to simulate and understand the magnetization and heat capacity curves of the pseudobinary Tb$_x$Pr$_{1-x}$Al$_2$, with $x = 0.10$ and 0.25, as a function of temperature. From the Rietveld analysis, we concluded that no crystallographic transition occurs in these samples, and the high symmetry of the magnetic structure was confirmed. Moreover, the different contributions from the reflection planes could be related to the known exchange bias-like effect characteristic for the $x = 0.25$ sample, also suggesting the existence of some rearrangement of the magnetic moments or even the presence of spin frustration in this system. Finally, the obtained set of theoretical parameters using the mean field approach for the two systems consisting of two sublattices allowed the experimental data to be described and to explain their physical behaviors. The ensemble of our results leads us to affirm that the quadrupolar interactions as well as an existence of some rearrangement of the magnetic moments or a frustration play an important role in the strong unidirectional anisotropy and the exchange bias-like effect observed in this pseudobinary system.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, University of Copenhagen, Brazilian Synchrotron Light Laboratory, Rutherford Appleton Laboratory, Helmholtz-Zentrum Berlin für Materialien und Energie, Technische Universität München, University of Campinas
Authors: Tedesco, J. C. G. (Ekstern), Carvalho, A. M. G. (Ekstern), Christensen, N. B. (Intern), Kockelmann, W. (Ekstern), Telling, M. T. F. (Ekstern), Yokaichiya, F. (Ekstern), Toebbens, D. M. (Ekstern), Simeoni, G. G. (Ekstern), Cardoso, L. P. (Ekstern), Coelho, A. A. (Ekstern), Bordallo, H. N. (Ekstern)
Number of pages: 9
Pages: 2884-2892
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Materials Science
Volume: 50
Issue number: 7
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
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.963 SNIP 1.388 CiteScore 2.54
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.926 SNIP 1.451 CiteScore 2.36
ISI indexed (2013): ISI indexed yes
We report angle resolved characterization of nanostructured and conventionally textured silicon solar cells. The nanostructured solar cells are realized through a single step, mask-less, scalable reactive ion etching (RIE) texturing of the surface. Photovoltaic properties including short circuit current, open circuit voltage, fill factor (FF) and power conversion efficiency are each measured as function of the relative incident angle between the solar cell and the light source. The relative incident angle is varied from 0° to 90° in steps of 10° in orthogonal axes, such that each solar cell is characterized at 100 different angle combinations. The angle resolved photovoltaic properties are summarized in terms of the average, angle-dependent electrical power output normalized to the power output at normal incidence and differently textured cells on different silicon substrates are compared in terms of angle resolved performance. The results show a 3% point improvement in average electrical power output normalized with respect to normal incidence power output of RIE textured, multicrystalline Si cells compared to conventional multicrystalline Si cells and above 1% point improvement of RIE textured monocrystalline Si cells compared to conventional monocrystalline Si cells.
Anharmonic stabilization and band gap renormalization in the perovskite CsSnI$_3$

Amongst the X(Sn,Pb)Y$_3$ perovskites currently under scrutiny for their photovoltaic applications, the cubic B–α phase of CsSnI$_3$ is arguably the best characterized experimentally. Yet, according to the standard harmonic theory of phonons, this deceptively simple phase should not exist at all due to rotational instabilities of the SnI$_6$ octahedra. Here, employing self-consistent phonon theory, we show that these soft modes are stabilized at experimental conditions through anharmonic phonon-phonon interactions between the Cs ions and their iodine cages. We further calculate the renormalization of the electronic energies due to vibrations and find an unusual opening of the band gap, estimated as 0.24 and 0.11 eV at 500 and 300 K, which we attribute to the stretching of Sn–I bonds. Our work demonstrates the important role of temperature in accurately describing these materials.

General information
State: Published
Organisations: Center for Atomic-scale Materials Design, Department of Physics
Authors: Patrick, C. (Intern), Jacobsen, K. W. (Intern), Thygesen, K. S. (Intern)
Number of pages: 5
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Journal: Physical Review B
Volume: 92
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Web of Science (2018): Indexed yes
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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
Anomalous magnetic structure and spin dynamics in magnetoelectric LiFePO$_4$

We report significant details of the magnetic structure and spin dynamics of LiFePO$_4$ obtained by single-crystal neutron scattering. Our results confirm a previously reported collinear rotation of the spins away from the principal $b$ axis, and they determine that the rotation is toward the $a$ axis. In addition, we find a significant spin-canting component along $c$. The possible causes of these components are discussed, and their significance for the magnetoelectric effect is analyzed. Inelastic neutron scattering along the three principal directions reveals a highly anisotropic hard plane consistent with earlier susceptibility measurements. Using a spin Hamiltonian, we show that the spin dimensionality is intermediate between $XY$- and Ising-like, with an easy $b$ axis and a hard $c$ axis. It is shown that both next-nearest neighbor exchange couplings in the $bc$ plane are in competition with the strongest nearest neighbor coupling.
Anomalous Particle Size Dependence of Magnetic Relaxation Phenomena in Goethite Nanoparticles

By use of Mossbauer spectroscopy we have studied the magnetic properties of samples of goethite nanoparticles with different particle size. The spectra are influenced by fluctuations of the magnetization directions, but the size dependence is not in accordance with the Neel-Brown expression for superparamagnetic relaxation of the magnetization vectors of the particles as a whole. The data suggest that the magnetic fluctuations can be explained by fluctuations of the magnetization directions of small interacting grains within the particles.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Research Centre Julich (FZJ)
Authors: Frandsen, C. (Intern), Madsen, D. E. (Intern), Boothroyd, C. B. (Ekstern), Mørup, S. (Intern)
Number of pages: 5
Pages: 481-485
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Main Research Area: Technical/natural sciences

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Issue number: 4
ISSN (Print): 0011-1643
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BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 0.347 SJR 0.19 CiteScore 0.65
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.297 SNIP 0.592
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.211 SNIP 0.558 CiteScore 0.79
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.214 SNIP 0.503 CiteScore 0.7
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.218 SNIP 0.35 CiteScore 0.66
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.246 SNIP 0.469 CiteScore 0.66
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.283 SNIP 0.511 CiteScore 0.77
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.281 SNIP 0.572
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.308 SNIP 0.634
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.278 SNIP 0.539
Scopus rating (2007): SJR 0.35 SNIP 0.716
Scopus rating (2006): SJR 0.32 SNIP 0.887
Scopus rating (2005): SJR 0.381 SNIP 0.949
Scopus rating (2004): SJR 0.348 SNIP 0.823
Scopus rating (2003): SJR 0.335 SNIP 0.693
Scopus rating (2002): SJR 0.347 SNIP 0.596
Scopus rating (2001): SJR 0.253 SNIP 0.503
Scopus rating (2000): SJR 0.362 SNIP 0.703
Scopus rating (1999): SJR 0.304 SNIP 0.535
A Numerical Analysis of Phononic-Assisted Control of Ultrasound Waves in Acoustofluidic Device

The ability to precisely sort individual microparticles/cells/droplets in suspension is important for various chemical and biological applications such as cancer cell detection, drug screening etc. The past decade, label-free particle handling of particle suspensions by ultrasonic radiation forces and streaming has received much attention, since it relies solely on mechanical properties such as particle size and contrast in density and compressibility. We present a theoretical study of phononic-assisted control of ultrasound waves in acoustofluidic devices. We propose the use of phononic crystal diffractors, which can be introduced in acoustofluidic structures. These diffractors can be applied in the design of efficient resonant cavities, directional sound waves for new types of particle sorting methods, or acoustically controlled deterministic lateral displacement. The PnC-diffractor-based devices can be made configurable, by embedding the diffractors, all working at the same excitation frequency but with different resulting diffraction patterns, in exchangeable membranes on top of the device.

General information
State: Published
Organisations: Department of Physics, Biophysics and Fluids
Authors: Moiseyenko, R. (Intern), Bruus, H. (Intern)
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Conference: 2015 International Congress on Ultrasonics, Metz, France, 10/05/2015 - 10/05/2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Physics Procedia
Volume: 70
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Scopus rating (2017): SNIP 0.614 SJR 0.351 CiteScore 0.67
Scopus rating (2016): CiteScore 0.65 SJR 0.347 SNIP 0.574
Scopus rating (2015): SJR 0.262 SNIP 0.572 CiteScore 0.61
Scopus rating (2014): SJR 0.401 SNIP 0.696 CiteScore 0.78
Scopus rating (2013): SJR 0.29 SNIP 0.605 CiteScore 0.72
ISI indexed (2013): ISI indexed no
Scopus rating (2012): SJR 0.28 SNIP 0.623 CiteScore 0.5
ISI indexed (2012): ISI indexed no
Web of Science (2012): Indexed yes
Scopus rating (2011): SJR 0.227 SNIP 0.467 CiteScore 0.45
ISI indexed (2011): ISI indexed no
Scopus rating (2010): SJR 0.218 SNIP 0.318
Scopus rating (2009): SJR 0.202 SNIP 0.456
Original language: English
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Publication: Research - peer-review › Conference article – Annual report year: 2015

Application of Generalized Mie Theory to EELS Calculations as a Tool for Optimization of Plasmonic Structures

Technical applications of plasmonic nanostructures require a careful structural optimization with respect to the desired functionality. The success of such optimizations strongly depends on the applied method. We extend the generalized multiparticle Mie (GMM) computational electromagnetic method and use it to excite a system of plasmonic nanoparticles with an electron beam. This method is applied to EELS calculations of a gold dimer and compared to other methods. It is demonstrated that the GMM method is so efficient, that it can be used in the context of structural optimization by the
application of genetic algorithms combined with a simplex algorithm. The scheme is applied to the design of plasmonic filters.

**General information**

State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Max Planck Institute, Martin-Luther University, Humboldt-University of Berlin, University of Bremen, Institut für Werkstofftechnik
Authors: Thomas, S. (Ekstern), Matyssek, C. (Ekstern), Hergert, W. (Ekstern), Arnold, M. (Ekstern), Kiewidt, L. (Ekstern), Karamehmedovic, M. (Intern), Wriedt, T. (Ekstern)
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Pages: 865-874
Publication date: 2015
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**Publication information**

Journal: Plasmonics
Volume: 11
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ISSN (Print): 1557-1955
Ratings:
- BFI (2018): BFI-level 1
- Web of Science (2018): Indexed yes
- BFI (2017): BFI-level 1
- Scopus rating (2017): SNIP 0.791 SJR 0.679 CiteScore 2.13
- Web of Science (2017): Indexed Yes
- BFI (2016): BFI-level 1
- Scopus rating (2016): CiteScore 1.8 SJR 0.635 SNIP 0.701
- Web of Science (2016): Indexed yes
- BFI (2015): BFI-level 1
- Scopus rating (2015): SJR 0.755 SNIP 0.824 CiteScore 2.07
- Web of Science (2015): Indexed yes
- BFI (2014): BFI-level 1
- Scopus rating (2014): SJR 0.93 SNIP 0.925 CiteScore 2.32
- Web of Science (2014): Indexed yes
- BFI (2013): BFI-level 1
- Scopus rating (2013): SJR 1.179 SNIP 1.23 CiteScore 2.85
- ISI indexed (2013): ISI indexed yes
- Web of Science (2013): Indexed yes
- BFI (2012): BFI-level 1
- Scopus rating (2012): SJR 1.223 SNIP 0.943 CiteScore 2.73
- ISI indexed (2012): ISI indexed yes
- Scopus rating (2011): SJR 1.274 SNIP 1.394 CiteScore 3.12
- ISI indexed (2011): ISI indexed yes
- Scopus rating (2010): SJR 2.001 SNIP 1.727
- Web of Science (2010): Indexed yes
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**A reusable device for electrochemical applications of hydrogel supported black lipid membranes**

Black lipid membranes (BLMs) are significant in studies of membrane transport, incorporated proteins/ion transporters, and hence in construction of biosensor devices. Although BLMs provide an accepted mimic of cellular membranes, they
are inherently fragile. Techniques are developed to stabilize them, such as hydrogel supports. In this paper, we present a reusable device for studies on hydrogel supported (hs) BLMs. These are formed across an ethylene tetrafluoroethylene (ETFE) aperture array supported by the hydrogel, which is during in situ polymerization covalently “sandwiched” between the ETFE substrate and a gold electrode microchip, thus allowing direct electrochemical studies with the integrated working electrodes. Using electrochemical impedance spectroscopy (EIS), X-ray photoelectron spectroscopy and contact angle measurements, we demonstrate the optimized chemical modifications of the gold electrode microchips and plasma modification of the ETFE aperture arrays facilitating covalent “sandwiching” of the hydrogel. Both fluorescence microscopy and EIS were used to demonstrate the induced spontaneous thinning of a deposited lipid solution, leading to formation of stabilized hsBLMs on average in 10 min. The determined specific membrane capacitance and resistance were shown to vary in the range 0.31-0.49 μF/cm² and 45-65 kΩ cm², respectively, corresponding to partially solvent containing BLMs with an average life time of 60-80 min. The characterized hsBLM formation and devised equivalent circuit models lead to a schematic model to illustrate lipid molecule distribution in hydrogel-supported apertures. The functionality of stabilized hsBLMs and detection sensitivity of the platform were verified by monitoring the effect of the ion transporter valinomycin.

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Assessments of macroscopicity for quantum optical states

With the slow but constant progress in the coherent control of quantum systems, it is now possible to create large quantum superpositions. There has therefore been an increased interest in quantifying any claims of macroscopicity. We attempt here to motivate three criteria which we believe should enter in the assessment of macroscopic quantumness: The number of quantum fluctuation photons, the purity of the states, and the ease with which the branches making up the state can be distinguished. © 2014.
Back-illuminated Si photocathode: a combined experimental and theoretical study for photocatalytic hydrogen evolution

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Band-gap engineering of functional perovskites through quantum confinement and tunneling

An optimal band gap that allows for a high solar-to-fuel energy conversion efficiency is one of the key factors to achieve sustainability. We investigate computationally the band gaps and optical spectra of functional perovskites composed of layers of the two cubic perovskite semiconductors BaSnO3 and BaTaO2N. Starting from an indirect gap of around 3.3 eV for BaSnO3 and a direct gap of 1.8 eV for BaTaO2N, different layerings can be used to design a direct gap of the functional perovskite between 2.3 and 1.2 eV. The variations of the band gap can be understood in terms of quantum confinement and tunneling. We also calculate the light absorption of the different heterostructures and demonstrate a large sensitivity to the detailed layering.
Benchmarking Pt-based electrocatalysts for low temperature fuel cell reactions with the rotating disk electrode: Oxygen reduction and hydrogen oxidation in the presence of CO

We present up-to-date benchmarking methods for testing electrocatalysts for polymer exchange membrane fuel cells (PEMFC), using the rotating disk electrode (RDE) method. We focus on the oxygen reduction reaction (ORR) and the hydrogen oxidation reaction (HOR) in the presence of CO. We have chosen our experimental methods to provide the most optimal compromise between the ease of carrying out the measurements and for ensuring comparability with PEMFC conditions. For the ORR, the effect of temperature, scan rate, Ohmic drop correction and background subtraction on the catalyst activity is investigated, both on a polycrystalline Pt disk and two different commercial Pt/C catalysts. To benchmark the CO tolerance of HOR catalysts, cyclic voltammetry and chronoamperometry are used, on polycrystalline Pt and commercial catalysts consisting of Pt/C and PtRu/C. We recommend the optimal conditions for obtaining a benchmark of ORR activity and CO tolerance of HOR catalysts.

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Bifurcation Analysis of Structures in a Convection Model

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Broad spectrum moderators and advanced reflector filters using $^{208}$Pb

Cold and thermal neutrons used in neutrons scattering experiments are produced in nuclear reactors and spallation sources. The neutrons are cooled to thermal or cold temperatures in thermal and cold moderators, respectively. The present study shows that it is possible to exploit the poor thermalizing property of $^{208}$Pb to design a broad spectrum moderator, i.e. a moderator which emits thermal and cold neutrons from the same position. Using $^{208}$Pb as a reflector filter material is shown to be slightly less efficient than a conventional beryllium reflector filter. However, when surrounding the reflector filter by a cold moderator it is possible to regain the neutrons with wavelengths below the Bragg edge, which are suppressed in the beryllium reflector filter. In both the beryllium and lead case surrounding the reflector filter with a cold moderator increases the cold brightness significantly compared to a conventional reflector filter.

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Bulk Ion Heating with ICRF Waves in Tokamaks

Heating with ICRF waves is a well-established method on present-day tokamaks and one of the heating systems foreseen for ITER. However, further work is still needed to test and optimize its performance in fusion devices with metallic high-Z plasma facing components (PFCs) in preparation of ITER and DEMO operation. This is of particular importance for the bulk ion heating capabilities of ICRF waves. Efficient bulk ion heating with the standard ITER ICRF scheme, i.e. the second harmonic heating of tritium with or without 3He minority, was demonstrated in experiments carried out in deuterium-tritium plasmas on JET and TFTR and is confirmed by ICRF modelling. This paper focuses on recent experiments with 3He minority heating for bulk ion heating on the ASDEX Upgrade (AUG) tokamak with ITER-relevant all-tungsten PFCs. An increase of 80% in the central ion temperature Ti from 3 to 5.5 keV was achieved when 3 MW of ICRF power tuned to the central 3He ion cyclotron resonance was added to 4.5 MW of deuterium NBI. The radial gradient of the Ti profile reached locally values up to about 50 keV/m and the normalized logarithmic ion temperature gradients R/LTi of about 20, which are unusually large for AUG plasmas. The large changes in the Ti profiles were accompanied by significant changes in measured plasma toroidal rotation, plasma impurity profiles and MHD activity, which indicate concomitant changes in plasma properties with the application of ICRF waves. When the 3He concentration was increased above the optimum range for bulk ion heating, a weaker peaking of the ion temperature profile was observed, in line with theoretical expectations.

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Calculated optical absorption of different perovskite phases

We present calculations of the optical properties of a set of around 80 oxides, oxynitrides, and organometal halide cubic and layered perovskites (Ruddlesden-Popper and Dion-Jacobson phases) with a bandgap in the visible part of the solar spectrum. The calculations show that for different classes of perovskites the solar light absorption efficiency varies greatly depending not only on bandgap size and character (direct/indirect) but also on the dipole matrix elements. The oxides exhibit generally a fairly weak absorption efficiency due to indirect bandgaps while the most efficient absorbers are found in the classes of oxynitride and organometal halide perovskites with strong direct transitions.
Catalysts, Protection Layers, and Semiconductors: The Challenge of Interfacing

Hydrogen is the simplest solar fuel to produce and in this presentation we shall give a short overview of the pros and cons of various tandem devices [1]. The large band gap semiconductor needs to be in front, but apart from that we can chose to have either the anode in front or back using either acid or alkaline conditions. Since most relevant semiconductors are very prone to corrosion the advantage of using buried junctions and using protection layers offering shall be discussed [2-4]. Next we shall discuss the availability of various catalysts for being coupled to these protections layers and how their stability may be evaluated [5, 6]. Examples of half-cell reaction using protection layers for both cathode and anode will be discussed though some of recent examples under both alkaline and acidic conditions. Si is a very good low band gap semiconductor and by using TiO2 as a protection layer we can stabilize it for both H2 and O2 evolution [7, 8, 9, 10]. Notably NiOx promoted by iron is a material that is transparent, providing protection, and is a good catalyst for O2 evolution. We have also recently started searching for large band gap semiconductors like III-V based or pervoskite materials and follow the same strategy by using protection layers and catalysts [11].
Cavitation inception from bubble nuclei

The tensile strength of ordinary water such as tap water or seawater is typically well below 1 bar. It is governed by cavitation nuclei in the water, not by the tensile strength of the water itself, which is extremely high. Different models of the nuclei have been suggested over the years, and experimental investigations of bubbles and cavitation inception have been presented. These results suggest that cavitation nuclei in equilibrium are gaseous voids in the water, stabilized by a skin which allows diffusion balance between gas inside the void and gas in solution in the surrounding liquid. The cavitation nuclei may be free gas bubbles in the bulk of water, or interfacial gaseous voids located on the surface of particles in the water, or on bounding walls. The tensile strength of these nuclei depends not only on the water quality but also on the pressure-time history of the water. A recent model and associated experiments throw new light on the effects of transient pressures on the tensile strength of water, which may be notably reduced or increased by such pressure changes.
Cavitation nuclei in water exposed to transient pressures

A model of skin-stabilized interfacial cavitation nuclei and their response to tensile and compressive stressing is presented. The model is evaluated in relation to experimental tensile strength results for water at rest at the bottom of an open water-filled container at atmospheric pressure and room temperature. These results are obtained by recording the initial growth of cavities generated by a short tensile pulse applied to the bottom of the container. It is found that the cavitation nuclei shift their tensile strength depending on their pressure history. Static pressurization for an extended period of time prior to testing is known to increase the tensile strength of water, but little information is available on how it is affected by compression pulses of short duration. This is addressed by imposing compression pulses of approximately 1 ms duration and a peak intensity of a few bar prior to the tension pulse. The observations are interpreted on the basis of the new model.
We show experimentally as well as theoretically that patterned magnetic tunnel junctions can be characterized using the current-in-plane tunneling (CIPT) method, and the key parameters, the resistance-area product (RA) and the tunnel magnetoresistance (TMR), can be determined. The CIPT method relies on four-point probe measurements performed with a range of different probe pitches and was originally developed for infinite samples. Using the method of images, we derive a modified CIPT model, which compensates for the insulating boundaries of a finite rectangular sample geometry. We measure on square tunnel junction pads with varying sizes and analyze the measured data using both the original and the modified CIPT model. Thus, we determine in which sample size range the modified CIPT model is needed to ensure validity of the extracted sample parameters, RA and TMR. In addition, measurements as a function of position on a square tunnel junction pad are used to investigate the sensitivity of the measurement results to probe misalignment.
Characterization of nano-textured samples in a production environment

Nano-textured surfaces have been characterized by optical diffraction techniques using an adapted commercial light microscope with two detectors, a CCD camera and a spectrometer. We demonstrate that the microscope has a resolution in the nanometer range, also in an environment with many vibrations, such as a machine floor. The acquisition and analysing time for the topological parameters height, width and sidewall angle is only a few milliseconds.

It is demonstrated that by simple adaptions to an optical microscope we can measure nano-textured surfaces with an uncertainty of a few nanometers for the height and width of the structures. The microscope has been validated by measuring on certified transfer artefact and 1D gratings. The measurements are very robust, such that vibrations of the sample and/or the microscope do not affect the results. The sample can be translated during acquisition, as long as the beam spot is kept inside an area with homogenous structures, which makes the proposed microscope well suited for implementation in a production environment.

Characterization of positional errors and their influence on micro four-point probe measurements on a 100 nm Ru film

Thin-film sheet resistance measurements at high spatial resolution and on small pads are important and can be realized with micrometer-scale four-point probes. As a result of the small scale the measurements are affected by electrode position errors. We have characterized the electrode position errors in measurements on Ru thin film using an Au-coated 12-point probe. We show that the standard deviation of the static electrode position error is on the order of 5 nm, which significantly affects the results of single configuration measurements. Position-error-corrected dual-configuration measurements, however, are shown to eliminate the effect of position errors to a level limited either by electrical measurement noise or dynamic position errors. We show that the probe contact points remain almost static on the surface during the measurements (measured on an atomic scale) with a standard deviation of the dynamic position errors of 3 Å. We demonstrate how to experimentally distinguish between different sources of measurement errors, e.g. electrical measurement noise, probe geometry error as well as static and dynamic electrode position errors.

Cocatalyst Designing: A Regenerable Molybdenum-Containing Ternary Cocatalyst System for Efficient Photocatalytic Water Splitting

Earth-abundant materials are required to facilitate upscaling of renewable hydrogen generation. Here, the synthesis of a novel oxidic ternary cocatalyst containing molybdenum, chromium, and copper, which has been found to be highly active in the overall photocatalytic splitting of water over gallium oxide, is described. With the noble metal-free system, requiring hydrogen evolution rates comparable to that of the well-established RhxCr2-xO3/Ga2O3 water splitting cocatalyst is achieved. Although the stability of the as-prepared ternary cocatalyst system appeared to be poor, the cocatalyst can be easily regenerated and stabilized by an oxygen treatment under ambient conditions. Furthermore, higher MoOx loadings were found to be more active and showed improved stability. By means of careful characterization using X-ray-based spectroscopy and TEM, the function of the individual cocatalyst compounds was closely examined, suggesting synergetic interactions of molybdena and chromia stabilizing CuO against photoreduction. Although stability issues should be further addressed, this work highlights that multicomponent systems, which are well-studied in industrial processes for heterogeneous reactions and commonly used in various other fields of research, can be used in solar water splitting. In particular, molybdena-containing materials are discovered as a new class of earth-abundant cocatalysts for overall water-splitting.
Co-existing hidden attractors in a radio-physical oscillator system

The term 'hidden attractor' relates to a stable periodic, quasiperiodic or chaotic state whose basin of attraction does not overlap with the neighborhood of an unstable equilibrium point. Considering a three-dimensional oscillator system that does not allow for the existence of an equilibrium point, this paper describes the formation of several different coexisting sets of hidden attractors, including the simultaneous presence of a pair of coinciding quasiperiodic attractors and of two mutually symmetric chaotic attractors. We follow the dynamics of the system as a function of the basic oscillator frequency, describe the bifurcations through which hidden attractors of different type arise and disappear, and illustrate the form of the basins of attraction.
In this article we have used the 2D fluid turbulence numerical model, ESEL, to simulate turbulent transport in edge tokamak plasma. Basic plasma parameters from the ASDEX Upgrade and COMPASS tokamaks are used as input for the model, and the output is compared with experimental observations obtained by reciprocating probe measurements from the two machines. Agreements were found in radial profiles of mean plasma potential and temperature, and in a level of density fluctuations. Disagreements, however, were found in the level of plasma potential and temperature fluctuations. This implicates a need for an extension of the ESEL model from 2D to 3D to fully resolve the parallel dynamics, and the coupling from the plasma to the sheath.

Comparison between 2D turbulence model ESEL and experimental data from AUG and COMPASS tokamaks

In this article we have used the 2D fluid turbulence numerical model, ESEL, to simulate turbulent transport in edge tokamak plasma. Basic plasma parameters from the ASDEX Upgrade and COMPASS tokamaks are used as input for the model, and the output is compared with experimental observations obtained by reciprocating probe measurements from the two machines. Agreements were found in radial profiles of mean plasma potential and temperature, and in a level of density fluctuations. Disagreements, however, were found in the level of plasma potential and temperature fluctuations. This implicates a need for an extension of the ESEL model from 2D to 3D to fully resolve the parallel dynamics, and the coupling from the plasma to the sheath.

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Comparison between the Oxygen Reduction Reaction Activity of Pd$_5$Ce and Pt$_5$Ce: The Importance of Crystal Structure

A set of electrochemical and X-ray spectroscopy measurements have been used conjointly with density functional theory (DFT) simulations to study the activity and stability of Pd$_5$Ce for the oxygen reduction reaction. A polycrystalline Pd$_5$Ce rod has been selected as a model catalyst to test if results on a several-fold activity increase of a series of Pt/rare-earth alloys hold also for Pd rare-earth alloys. Pd$_5$Ce crystallizes in two phases, a so-called low-temperature phase, L-Pd$_5$Ce, which has a cubic symmetry, and a high-temperature phase, H-Pd$_5$Ce, with a hexagonal symmetry. In both cases, a several-layers-thick Pd skin forms on the surface. Preliminary DFT results show that Pd overlayers under $\geq 2\%$ compressive strain should be more active than Pt. In L-Pd$_5$Ce, the overlayer is under tensile strain, whereas in H-Pd$_5$Ce (a structure similar to Pt$_5$Ce), it is under compressive strain. We have confirmed that in our sample, L-Pd$_5$Ce is the dominant phase, both in the bulk and the outermost layers, while a H-Pd$_5$Ce-like phase is also present as a minor component far below the surface. Electrochemical ORR assessments show that the Pd overlayer in Pd$_5$Ce is less active than the polycrystalline Pd sample, in agreement with DFT results for the L-Pd$_5$Ce phase. Although we did not discover a new promising Pd-based catalyst, we have shown that the activity for oxygen reduction is strongly influenced by the alloy crystal structure. Furthermore, we have qualitatively demonstrated that transformation from H-Pd$_5$Ce to L-Pd$_5$Ce is more facile, requires less atom rearrangement, than transformation from Pt$_5$Ce to Pt$_3$Ce, which might explain the kinetic stability of Pt$_5$Ce at low temperatures.
Comparison of the performance of cop-coated and Pt-coated radial junction n+p-silicon microwire-array photocathodes for the sunlight-driven reduction of water to H₂(g)

The electrocatalytic performance for hydrogen evolution has been evaluated for radial-junction n+p-Si microwire (MW) arrays with Pt or cobalt phosphide, CoP, nanoparticulate catalysts in contact with 0.50 M H₂SO₄(aq). The CoP-coated (2.0 mg cm⁻²) n+p-Si MW photocathodes were stable for over 12 h of continuous operation and produced an open-circuit photovoltage (V_oc) of 0.48 V, a light-limited photocurrent density (J_ph) of 17 mA cm⁻², a fill factor (ff) of 0.24, and an ideal regenerative cell efficiency (ηIRC) of 1.9% under simulated 1 Sun illumination. Pt-coated (0.5 mg cm⁻²) n+p-Si MW-array photocathodes produced V_oc = 0.44 V, J_ph = 14 mA cm⁻², ff = 0.46, and η = 2.9% under identical conditions. Thus, the MW geometry allows the fabrication of photocathodes entirely comprised of earth-abundant materials that exhibit performance comparable to that of devices that contain Pt.
We have studied the magnetic and superconducting properties of Ba(Fe$_{1-x}$Co$_x$)$_2$As$_2$ as a function of temperature and external magnetic field using neutron scattering and muon spin rotation. Below the superconducting transition temperature the magnetic and superconducting order parameters coexist and compete. A magnetic field can significantly enhance the magnetic scattering in the superconducting state, roughly doubling the Bragg intensity at 13.5 T. We perform a microscopic modelling of the data by use of a five-band Hamiltonian relevant to iron pnictides. In the superconducting state, vortices can slow down and freeze spin fluctuations locally. When such regions couple they result in a long-range ordered antiferromagnetic phase producing the enhanced magnetic elastic scattering in agreement with experiments.
We describe an emulsion-based preparation of patchy composite particles (diameter of 100-500 \( \mu \)m) consisting of a disclike epoxy core and a belt of porous polystyrene particles (diameter of 30 \( \mu \)m) with magnetite within the pores. Compared to the magnetically uniform polystyrene particles, the spontaneous aggregation of composite particles is suppressed when dispersed into liquid, which is attributed to the increased particle size, reduced magnetic susceptibility, and the shape of the magnetic domain distribution within the particles (spherical versus a belt). When the composite particles are coated by platinum-palladium layer we demonstrate they can be employed as switchable catalyst carriers, moving from one liquid phase to another when controlled by an external magnetic field.
We present a comprehensive first-principles study of the electronic structure of 51 semiconducting monolayer transition-metal dichalcogenides and -oxides in the 2H and 1T hexagonal phases. The quasiparticle (QP) band structures with spin-orbit coupling are calculated in the G(0)W(0) approximation, and comparison is made with different density functional theory descriptions. Pitfalls related to the convergence of GW calculations for two-dimensional (2D) materials are discussed together with possible solutions. The monolayer band edge positions relative to vacuum are used to estimate
the band alignment at various heterostructure interfaces. The sensitivity of the band structures to the in-plane lattice constant is analyzed and rationalized in terms of the electronic structure. Finally, the q-dependent dielectric functions and effective electron and hole masses are obtained from the QP band structure and used as input to a 2D hydrogenic model to estimate exciton binding energies. Throughout the paper we focus on trends and correlations in the electronic structure rather than detailed analysis of specific materials. All the computed data is available in an open database.

General information
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Organisations: Center for Atomic-scale Materials Design, Center for Nanostructured Graphene, Department of Physics
Authors: Rasmussen, F. A. (Intern), Thygesen, K. S. (Intern)
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Computational design of molecules for dye sensitized solar cells and nano electronics

The huge increase in computational power has enabled the use of high-throughput computational screening methods for many purposes. In combination with more detailed computational studies, this provides a powerful tool in the search for new materials and molecules useful for e.g. photovoltaics. This is illustrated in this thesis, where a high-throughput Density Functional Theory study of a total of 5145 porphyrin based dye molecules is presented. Initially, the structures of the dyes are optimized and the frontier energy orbital energies calculated. Following this, the dyes are scored for use in a dye sensitized solar cell (DSSC) in terms of a loss-less level alignment quality. This scoring only takes into account a simplified absorption spectrum of the dye in combination with the alignment between the molecular levels, the semi-conductor conduction band edge and the redox mediator. To improve on this, the effect of the free energy barrier associated with the dye regeneration reaction is included through extensive molecular dynamics simulations for a simple model dye, followed by an extrapolation of the result to the 5145 porphyrins. This model succeeds in rediscovering high efficiency dyes and suggests that the next generation of high efficiency porphyrin dyes may utilize a titanium metal center. Furthermore, the large internal reorganization energies calculated for the octahedral cobalt complexes, used as redox mediators, lead to the requirement of a large driving force for the regeneration reaction. Hence, using redox mediators with a lower internal reorganization energy would allow for a less constrained choice of dye, possibly boosting the efficiency. The obtained data is furthermore used to search for suitable pairs of porphyrins for a novel type of DSSC schemes, using two dyes in a molecular two-photon tandem approach. Here, a high current is sacrificed for a larger voltage. As a smaller current is however often associated with a better fill-factor, the proposed scheme may lead to an increase in the efficiency. Specific candidates for the different schemes are identified and the resulting setups have theoretically obtainable open-circuit voltages exceeding 1.5 V.

Creating a metal-molecule-metal junction allows tuning the conductance through the junction by manipulating the molecular energy levels. In this thesis a computational approach to model the conductance as a function of the applied bias voltage, shifting the molecular levels, for a redox active molecule is presented and compared to experimental results. Here, it is shown that shifting the molecular energy levels in and out of resonance with the Fermi level of the electrodes, allows for a standard tuning of the conductance. In addition to this, reversibly changing the redox state, allows for switching quantum interference on and off, shifting the conductance by an order of magnitude. The simple computational model used is furthermore qualitatively found to be in very good agreement with experiments.

A different way of tuning the conductance through a molecular junction, is by controlling the junction geometry. This is achieved by designing a molecule with two sets of anchor groups, which bind to gold with significantly different strengths. Hence, it is proposed that the geometry can be controlled by chemical passivisation of one type of anchor group. Using a simple computational model, this experimental hypothesis is verified and the change in conductance upon changing junction geometry is reproduced.

General information
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Organisations: Department of Physics, Theoretical Atomic-scale Physics
Authors: Ørnsø, K. B. (Intern), Thygesen, K. S. (Intern), Jacobsen, K. W. (Intern)
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Computational Discovery of Sustainable Energy Materials

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Organisations: Department of Physics, Theoretical Atomic-scale Physics
Authors: Thygesen, K. S. (Intern)
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Computational Screening of Energy Materials

The current energy consumption of the world's population relies heavily on fossil fuels. Unfortunately, the consumption of fossil fuels not only results in the emission of greenhouse gases which have deleterious effects on the environment but also the fossil fuel reserve is limited. Therefore, it is the need of the hour to search for environmentally benign renewable energy resources. The biggest source of the renewable energy is our sun and the immense energy it provides can be used to power the whole planet. However, an efficient way to harvest the solar energy to meet all the energy demand has not been realized yet.

A promising way to utilize the solar energy is the photon assisted water splitting. The process involves the absorption of sunlight with a semiconducting material (or a photoabsorber) and the generated electron-hole pair can be used to produce hydrogen by splitting the water. However, a single material cannot accomplish the whole process of the hydrogen evolution. In order to do so, a material should be able to absorb the sunlight and generate the electronhole pairs and evolve hydrogen at the cathode and oxygen at anode using the generated electron and hole respectively.

This thesis using first-principle calculations explores materials for the light absorption with the bandgap, band edge positions and the stability in aqueous conditions as descriptors. This strategy results in a handful of materials which can act as good photoabsorbers for the water splitting reaction. Additionally, strategies to tune the bandgap for different applications is also explored. To carry out the cathode reaction, two-dimensional metal dichalcogenides and oxides are explored with a suggestion of few potential candidates for the hydrogen evolution reaction.

The thermodynamics of all the above processes require an accurate description of the energies with the first-principle calculations. Therefore, along this line the accuracy and predictability of the Meta- Generalized Gradient Approximation functional with Bayesian error estimation is also assessed.

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Authors: Pandey, M. (Intern), Jacobsen, K. W. (Intern), Thygesen, K. S. (Intern)
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Concentration polarization: Electrodeposition and transport phenomena at overlimiting current

In the present thesis we study different aspects of concentration polarization, with emphasis on nonlinear transport phenomena and ramified electrode growth. We aim at extracting the essential features which characterize the problems, and to that end we employ a variety of numerical and analytical methods.

The initial study concerns a fundamental problem in the study of concentration polarization at overlimiting current, namely the emergence of an extended space-charge region near the ion-selective interface. Based on the so-called quasi-uniform charge density assumption (QUD), we develop an analytical model for the transport in a system with an extended space-charge region. By comparison with numerical simulations, we show that the analytical model captures all of the essential features of the problem. We use the model to derive a range of results characterizing the extended space-charge region. Secondly, we investigate concentration polarization in a microchannel with charged walls. We provide full numerical solutions to the transport problem, including the effects of advection and surface conduction in the electric double layers. We show that in large areas of the relevant parameter space the transport can be understood in terms of a group of simple analytical models. Some of these are generalizations of a previously published analytical model. In addition to the full numerical model, we employ a numerical boundary layer model with a slip velocity. By carefully comparing the full model and the boundary layer model, we reveal a number of issues, which invalidate most previous attempts at modeling microchannel concentration polarization using a slip model.

Returning to concentration polarization in a bulk system, we study the effects of water splitting at a permselective membrane. We investigate this coupled chemical and transport effect using two simple models of the reaction kinetics. The principal investigations are performed using numerical simulations, but in addition we derive an analytical model for the transport in the system. The analytical model reveals an important link between the current of salt ions and the current of water ions. This link seemingly exists independent of the specific reaction kinetics, and could help in furthering the understanding of the water splitting process. A fit of the model to experimental data from the literature shows quite good agreement, and provides some hints about the reaction kinetics in the given experiment.

In the final part of the thesis we investigate electrodeposition, and specifically the tendency of a cathode to become morphologically unstable and develop ramified growth. Firstly, we consider the stability of a flat metal electrode during electrodeposition. Using linear perturbation theory, we develop numerical and analytical models for the instability growth rate as a function of the instability wavelength. In contrast to previous work on the stability problem, our models apply at both under- and overlimiting current.

Secondly, we develop a numerical sharp-interface model describing the electrode growth. This model differs from the established phase-field models, in that it is applicable at overlimiting current and implements electrode reactions in a consistent way. Comparison of the sharp-interface model to the results of the stability analysis, provides a validation of the model behavior in the initial stages of the growth. Some preliminary results of the numerical simulations indicate that the electrodeposit morphology might be explainable in terms of a few key parameters.

General information
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Organisations: Department of Physics, Biophysics and Fluids
Authors: Nielsen, C. P. (Intern), Bruus, H. (Intern)
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Configurational Statistics of Magnetic Bead Detection with Magnetoresistive Sensors
Magnetic biosensors detect magnetic beads that, mediated by a target, have bound to a functionalized area. This area is often larger than the area of the sensor. Both the sign and magnitude of the average magnetic field experienced by the sensor from a magnetic bead depends on the location of the bead relative to the sensor. Consequently, the signal from multiple beads also depends on their locations. Thus, a given coverage of the functionalized area with magnetic beads does not result in a given detector response, except on the average, over many realizations of the same coverage. We present a systematic theoretical analysis of how this location-dependence affects the sensor response. The analysis is done for beads magnetized by a homogeneous in-plane magnetic field. We determine the expected value and standard deviation of the sensor response for a given coverage, as well as the accuracy and precision with which the coverage can be determined from a single sensor measurement. We show that statistical fluctuations between samples may reduce the sensitivity and dynamic range of a sensor significantly when the functionalized area is larger than the sensor area. Hence, the statistics of sampling is essential to sensor design. For illustration, we analyze three important published cases for which statistical fluctuations are dominant, significant, and insignificant, respectively.
Consistency between real and synthetic fast-ion measurements at ASDEX Upgrade

Internally consistent characterization of the properties of the fast-ion distribution from multiple diagnostics is a prerequisite for obtaining a full understanding of fast-ion behavior in tokamak plasmas. Here we benchmark several absolutely-calibrated core fast-ion diagnostics at ASDEX Upgrade by comparing fast-ion measurements from collective Thomson scattering, fast-ion spectroscopy, and neutron rate detectors with numerical predictions from the TRANSP/NUBEAM transport code. We also study the sensitivity of the theoretical predictions to uncertainties in the plasma kinetic profiles. We find that theory and measurements generally agree within these uncertainties for all three diagnostics during heating phases with either one or two neutral beam injection sources. This suggests that the measurements can be described by the same model assuming classical slowing down of fast ions. Since the three diagnostics in the adopted configurations probe partially overlapping regions in fast-ion velocity space, this is also consistent with good internal agreement among the measurements themselves. Hence, our results support the feasibility of combining multiple diagnostics at ASDEX Upgrade to reconstruct the fast-ion distribution function in 2D velocity space.
Continuous Variable Quantum Key Distribution with a Noisy Laser

Existing experimental implementations of continuous-variable quantum key distribution require shot-noise limited operation, achieved with shot-noise limited lasers. However, loosening this requirement on the laser source would allow for cheaper, potentially integrated systems. Here, we implement a theoretically proposed prepare-and-measure continuous-variable protocol and experimentally demonstrate the robustness of it against preparation noise stemming for instance from technical laser noise. Provided that direct reconciliation techniques are used in the post-processing we show that for small distances large amounts of preparation noise can be tolerated in contrast to reverse reconciliation where the key rate quickly drops to zero. Our experiment thereby demonstrates that quantum key distribution with non-shot-noise limited laser diodes might be feasible.

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Organisations: Department of Physics, Quantum Physics and Information Technology
Authors: Jacobsen, C. S. (Intern), Gehring, T. (Intern), Andersen, U. L. (Intern)
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Journal: Entropy
This paper introduces the fundamental continuum theory governing momentum transport in isotropic nanofluidic systems. The theory is an extension of the classical Navier-Stokes equation, and includes coupling between translational and
rotational degrees of freedom as well as nonlocal response functions that incorporate spatial correlations. The continuum theory is compared with molecular dynamics simulation data for both relaxation processes and fluid flows, showing excellent agreement on the nanometer length scale. We also present practical tools to estimate when the extended theory should be used. It is shown that in the wall-fluid region the fluid molecules align with the wall, and in this region the isotropic model may fail and a full anisotropic description is necessary.
Controlling Electrical Conductance through a π-Conjugated Cruciform Molecule by Selective Anchoring to Gold Electrodes

Tuning charge transport at the single-molecule level plays a crucial role in the construction of molecular electronic devices. Introduced herein is a promising and operationally simple approach to tune two distinct charge-transport pathways through a cruciform molecule. Upon in situ cleavage of triisopropylsilyl groups, complete conversion from one junction type to another is achieved with a conductance increase by more than one order of magnitude, and it is consistent with predictions from ab initio transport calculations. Although molecules are well known to conduct through different orbitals (either HOMO or LUMO), the present study represents the first experimental realization of switching between HOMO- and LUMO-dominated transport within the same molecule.

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Organisations: Department of Physics, University of Bern
Authors: Huang, C. (Ekstern), Chen, S. (Ekstern), Ørnsø, K. B. (Intern), Reber, D. (Ekstern), Baghernejad, M. (Ekstern), Fu, Y. (Ekstern), Wandlowski, T. (Ekstern), Decurtins, S. (Ekstern), Hong, W. (Ekstern), Thygesen, K. S. (Intern), Liu, S. (Ekstern)
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BFI (2015): BFI-level 2
Controlling Electrical Conductance through a \( \pi \)-Conjugated Cruciform Molecule by Selective Anchoring to Gold Electrodes

Tuning charge transport at the single-molecule level plays a crucial role in the construction of molecular electronic devices. Introduced herein is a promising and operationally simple approach to tune two distinct charge-transport pathways through a cruciform molecule. Upon in situ cleavage of trisopropylsilyl groups, complete conversion from one junction type to another is achieved with a conductance increase by more than one order of magnitude, and it is consistent with predictions from ab initio transport calculations. Although molecules are well known to conduct through different orbitals (either HOMO or LUMO), the present study represents the first experimental realization of switching between HOMO- and LUMO-conducting pathways.
LUMO-dominated transport within the same molecule.

**General information**

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Organisations: Department of Physics, University of Bern
Authors: Huang, C. (Ekstern), Chen, S. (Ekstern), Ørnsø, K. B. (Intern), Reber, D. (Ekstern), Baghernejad, M. (Ekstern), Fu, Y. (Ekstern), Wandlowski, T. (Ekstern), Decurtins, S. (Ekstern), Hong, W. (Ekstern), Thygesen, K. S. (Intern), Liu, S. (Ekstern)
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**Controlling the Activity and Stability of Pt-Based Electrocatalysts By Means of the Lanthane 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-lanthane 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 PbGd 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.
Convergent evolution of vascular optimization in kelp (Laminariales)

Terrestrial plants and mammals, although separated by a great evolutionary distance, have each arrived at a highly conserved body plan in which universal allometric scaling relationships govern the anatomy of vascular networks and key functional metabolic traits. The universality of allometric scaling suggests that these phyla have each evolved an 'optimal' transport strategy that has been overwhelmingly adopted by extant species. To truly evaluate the dominance and universality of vascular optimization, however, it is critical to examine other, lesser-known, vascularized phyla. The brown algae (Phaeophyceae) are one such group—as distantly related to plants as mammals, they have convergently evolved a plant-like body plan and a specialized phloem-like transport network. To evaluate possible scaling and optimization in the kelp vascular system, we developed a model of optimized transport anatomy and tested it with measurements of the giant kelp, Macrocystis pyrifera, which is among the largest and most successful of macroalgae. We also evaluated three classical allometric relationships pertaining to plant vascular tissues with a diverse sampling of kelp species. Macrocystis pyrifera displays strong scaling relationships between all tested vascular parameters and agrees with our model; other species within the Laminariales display weak or inconsistent vascular allometries. The lack of universal scaling in the kelps and the presence of optimized transport anatomy in M. pyrifera raises important questions about the evolution of optimization and the possible competitive advantage conferred by optimized vascular systems to multicellular phyla.
Correction of complex nonlinear signal response from a pixel array detector

The pulsed free-electron laser light sources represent a new challenge to photon area detectors due to the intrinsic spontaneous X-ray photon generation process that makes single-pulse detection necessary. Intensity fluctuations up to 100% between individual pulses lead to high linearity requirements in order to distinguish small signal changes. In real detectors, signal distortions as a function of the intensity distribution on the entire detector can occur. Here a robust method to correct this nonlinear response in an area detector is presented for the case of exposures to similar signals. The method is tested for the case of diffuse scattering from liquids where relevant sub-1% signal changes appear on the same order as artifacts induced by the detector electronics.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, SLAC National Accelerator Laboratory
Authors: Brandt van Driel, T. (Intern), Herrmann, S. (Ekstern), Carini, G. (Ekstern), Nielsen, M. M. (Intern), Lemke, H. T. (Ekstern)
Correlating Structure and Oxygen Reduction Activity on Y/Pt(111) and Gd/Pt(111) Single Crystals
Polymer Electrolyte Membrane Fuel Cells (PEMFC) hold promise as a zero-emission source of power, particularly suitable for automotive vehicles. However, the high loading of Pt required to catalyse the Oxygen Reduction Reaction (ORR) at the PEMFC cathode prevents the commercialisation of this technology. Improving the activity of Pt by alloying it with other metals could decrease the loading of Pt at the cathode to a level comparable to Pt-group metal loading in internal combustion engines.

PtxY and PtxGd exhibit exceptionally high activity for oxygen reduction, both in the polycrystalline form and the nanoparticulate form. [1,2,3,4]. Moreover, their negative alloying energy may make them inherently less prone to degradation via dealloying than the more commonly investigated alloys of Pt and late transition metals such as Ni, Co, Fe and Cu. In order to understand the origin of the enhanced activity of these alloys, we have investigated Y/Pt(111) [5] and Gd/Pt(111) single crystals, formed by depositing large amounts of Y and Gd on Pt(111) single crystals under Ultra-High Vacuum (UHV) conditions and annealing to high temperatures. We subsequently characterised the surface using low energy electron diffraction, ion scattering spectroscopy and temperature programmed desorption of CO. After the characterization in UHV, the ORR activity was measured. Angle resolved X-ray photoelectron spectroscopy measurements were carried out after the electrochemical measurements. These experiments revealed, that thick platinum overlayers had been formed, and that the structure formed under reaction conditions was significantly different from our initial expectations. The structures of the overlayers were investigated using surface sensitive X-ray diffraction using synchrotron radiation, and correlated to the oxygen reduction activity.

Crystalline TiO2: A Generic and Effective Electron-Conducting Protection Layer for Photoanodes and -cathodes
Stabilizing efficient photoabsorbers for solar water splitting has recently shown significant progress with the development of various protection layers. Suitable protection layers for tandem devices should be conductive, transparent, and stable in strongly acidic or alkaline solutions. This paper shows that under certain conditions n-type semiconductors, such as TiO2, can be used as protection layers for Si-based photoanodes. It also provides evidence that even in a photoanode assembly TiO2 is conducting only electrons (not holes as in p-type protection layers), and therefore TiO2 can be described as a simple ohmic contact. This renders n-type semiconductors, such as TiO2, to be versatile and simple protection layers, which can be used for photoanodes and as previously shown for photocathodes. The ohmic behavior of n-type TiO2 in a Si/TiO2-photoanode assembly is demonstrated under dark and illuminated conditions by performing the oxygen evolution reaction (OER) and using the Fe(II)/Fe(III) redox couple. These measurements reveal that the performance of the Si/TiO2-photoanode assembly is strongly dependent on the TiO2/electrolyte interaction. Finally, the conditions and requirements that make TiO2 generally applicable for photoanode assemblies, and thus for protecting tandem devices, are outlined and quantitatively shown by band diagram calculations. The results presented here provide the understanding required for the design of highly efficient and stable photoelectrochemical water splitting devices.
Dark-field X-ray microscopy for multiscale structural characterization

Many physical and mechanical properties of crystalline materials depend strongly on their internal structure, which is typically organized into grains and domains on several length scales. Here we present dark-field X-ray microscopy; a non-destructive microscopy technique for the three-dimensional mapping of orientations and stresses on lengths scales from 100 nm to 1 mm within embedded sampling volumes. The technique, which allows ‘zooming’ in and out in both direct and angular space, is demonstrated by an annealing study of plastically deformed aluminium. Facilitating the direct study of the interactions between crystalline elements is a key step towards the formulation and validation of multiscale models that account for the entire heterogeneity of a material. Furthermore, dark-field X-ray microscopy is well suited to applied topics, where the structural evolution of internal nanoscale elements (for example, positioned at interfaces) is crucial to the performance and lifetime of macro-scale devices and components thereof.

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Scopus rating (2014): SJR 6.41 SNIP 3.034 CiteScore 10.77
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Scopus rating (2012): SJR 5.866 SNIP 2.829 CiteScore 8.32
Dark field X-ray microscopy for studies of recrystallization

We present the recently developed technique of Dark Field X-Ray Microscopy that utilizes the diffraction of hard X-rays from individual grains or subgrains at the (sub)micrometre-scale embedded within mm-sized samples. By magnifying the diffracted signal, 3D mapping of orientations and strains inside the selected grain is performed with an angular resolution of 0.005° and a spatial resolution of 200 nm. Furthermore, the speed of the measurements at high-intensity synchrotron facilities allows for fast non-destructive in situ determination of structural changes induced by annealing or other external influences. The capabilities of Dark Field X-Ray Microscopy are illustrated by examples from an ongoing study of recrystallization of 50% cold-rolled Al1050 specimens.
Deformation-induced orientation spread in individual bulk grains of an interstitial-free steel

Three-dimensional X-ray diffraction was employed to characterize the lattice rotations of individual bulk grains in a 9% tensile deformed sample of interstitial-free steel. Three grains of initially close orientation that are representative of the scatter of all investigated grains with tensile axes near <522> were identified. Their rotation paths and intragranular orientation spread were analysed in detail, using crystal plasticity modelling to evaluate the nature of the orientation spread. It was found that the same set of most stressed slip systems are active in the three grains and that variations in the relative activities of the two most stressed systems account for the dominant orientation spread in the grains. The distribution of slip on these systems varies from grain to grain and also within each grain. While the grain orientation controls the identity of these slip systems, the variations are attributed to grain boundary and grain interaction effects. © 2014 Acta Materialia Inc. Published by Elsevier Ltd. All rights reserved.
Scopus rating (2012): SJR 3.37 SNIP 2.875 CiteScore 4.28
ISI indexed (2012): ISI indexed yes
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Scopus rating (2011): SJR 3.215 SNIP 2.768 CiteScore 4.27
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Web of Science (2011): Indexed yes
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Scopus rating (2010): SJR 3.709 SNIP 2.698
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Scopus rating (2009): SJR 3.663 SNIP 2.625
Web of Science (2009): Indexed yes
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Scopus rating (2008): SJR 3.82 SNIP 2.774
Web of Science (2008): Indexed yes
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Scopus rating (2006): SJR 3.615 SNIP 3.118
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 3.22 SNIP 3.038
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Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 3.852 SNIP 3.258
Web of Science (2003): Indexed yes
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 3.198 SNIP 2.73
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Web of Science (2000): Indexed yes
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Relations
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Deformation-induced intragranular orientation spread in ferrite investigated by 3DXRD and forward modeling
Intragranular orientation spread induced by grain interaction
Grain-scale investigations of deformation and surface treatment of stainless steel
Projects:
Deformation-induced orientation spread in individual bulk grains of an interstitial-free steel
Source: PublicationPreSubmission
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Design of a solid state laser for low noise upconversion detection of near infrared light
To maximize signal-to-noise ratio for upconversion of near-infrared light we show that the mixing intensity should be 3 GW/m2. With emphasis on the noise contribution from random duty-cycle errors the optimum design parameters is discussed.

General information
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.
Detailed Characterization of a Nanosecond-Lived Excited State: X-ray and Theoretical Investigation of the Quintet State in Photoexcited [Fe(terpy)(2)](2+)

Theoretical predictions show that depending on the populations of the Fe 3d(xy), 3d(xz), and 3d(yz) orbitals two possible quintet states can exist for the high-spin state of the photoswitchable model system [Fe(terpy)(2)](2+). The differences in the structure and molecular properties of these B-5(2) and E-5 quintets are very small and pose a substantial challenge for experiments to resolve them. Yet for a better understanding of the physics of this system, which can lead to the design of novel molecules with enhanced photoswitching performance, it is vital to determine which high-spin state is reached in the transitions that follow the light excitation. The quintet state can be prepared with a short laser pulse and can be studied with cutting-edge time-resolved X-ray techniques. Here we report on the application of an extended set of X-ray spectroscopy and scattering techniques applied to investigate the quintet state of [Fe(terpy)(2)](2+) 80 ps after light excitation. High-quality X-ray absorption, nonresonant emission, and resonant emission spectra as well as X-ray diffuse scattering data clearly reflect the formation of the high-spin state of the [Fe(terpy)(2)](2+) molecule; moreover, extended X-ray absorption fine structure spectroscopy resolves the Fe-ligand bond-length variations with unprecedented bond-length accuracy in time-resolved experiments. With ab initio calculations we determine why, in contrast to most related systems, one configurational mode is insufficient for the description of the low-spin (LS)-high-spin (HS) transition. We identify the electronic structure origin of the differences between the two possible quintet modes, and finally, we unambiguously identify the formed quintet state as 5E, in agreement with our theoretical expectations.
Determination of Core-Shell Structures in Pd-Hg Nanoparticles by STEM-EDX

The structural and elemental configuration of a high-performing Pd-Hg electrocatalyst for oxygen reduction to hydrogen peroxide has been studied by means of high-resolution scanning transmission electron microscopy. Pd-Hg nanoparticles
are shown to have a crystalline core-shell structure, with a Pd core and a Pd-Hg ordered alloy shell. The ordered shell is responsible for the high oxygen reduction selectivity to H$_2$O$_2$.

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BFI (2015): BFI-level 1
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Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.89 SNIP 1.103 CiteScore 4.52
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
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ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
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**Determining fast-ion velocity-space distribution functions using velocity-space tomography**

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Organisations: Department of Physics, Plasma Physics and Fusion Energy, Max Planck Institute for Plasma Physics, University of California, Irvine, Uppsala University
Authors: Jacobsen, A. S. (Intern), Salewski, M. (Intern), Geiger, B. (Ekstern), Stagner, L. (Ekstern), Eriksson, J. (Ekstern), Nielsen, S. K. (Intern), Heidbrink, W. (Ekstern), Korsholm, S. B. (Intern), Leipold, F. (Intern), Rasmussen, J. (Intern), Pedersen, M. S. (Intern), Weiland, M. (Ekstern)
Development of 3D ferromagnetic model of tokamak core with strong toroidal asymmetry

Fully 3D model of strongly asymmetric tokamak core, based on boundary integral method approach (i.e. characterization of ferromagnet by its surface) is presented. The model is benchmarked on measurements on tokamak GOLEM, as well as compared to 2D axisymmetric core equivalent for this tokamak, presented in previous work. Linearized model well describes quantitative characteristics of BR field, generated by poloidal field coils located close to core central column, and distorted by ferromagnet. A discrepancy is seen between linearized form of model for BR field generated by coils under the transformer limbs and the measurements. Future work will thus include implementation of the non-linearity effects in order to further investigate this issue.
Development of Catalysts for ORR HT-PEMFCs

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Development of silicon based bottom cell for tandem photoelectrochemical water splitting device structures

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State: Published
Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics, Silicon Microtechnology
Authors: Bae, D. (Intern), Chorkendorff, I. (Intern), Hansen, O. (Intern), Vesborg, P. C. K. (Intern)
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12_04827_34_PhD_Thesis_Dowon_Bae.pdf_2273019_1_1.pdf
Direct observation of the dealloying process of a platinum–yttrium nanoparticle fuel cell cathode and its oxygenated species during the oxygen reduction reaction

Size-selected 9 nm Pt,Y nanoparticles have recently shown an outstanding catalytic activity for the oxygen reduction reaction, representing a promising cathode catalyst for proton exchange membrane fuel cells (PEMFCs). Studying their electrochemical dealloying is a fundamental step towards the understanding of both their activity and stability. Herein, size-selected 9 nm Pt,Y nanoparticles have been deposited on the cathode side of a PEMFC specifically designed for in situ ambient pressure X-ray photoelectron spectroscopy (APXPS). The dealloying mechanism was followed in situ for the first time. It proceeds through the progressive oxidation of alloyed Y atoms, soon leading to the accumulation of Y³⁺ cations at the cathode. Acid leaching with sulfuric acid is capable of accelerating the dealloying process and removing these Y³⁺ cations which might cause long term degradation of the membrane. The use of APXPS under near operating conditions allowed observing the population of oxygenated surface species as a function of the electrochemical potential. Similar to the case of pure Pt nanoparticles, non-hydrated hydroxide plays a key role in the ORR catalytic process.

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Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
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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
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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
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Web of Science (2011): Indexed yes
With the arrival of X-ray Free Electron Lasers (XFELs), 2D area detectors with a large dynamic range for detection of hard X-rays with fast readout rates are required for many types of experiments. Extracting the desired information from these detectors has been challenging due to unpredicted fluctuations in the measured images. For techniques such as time-resolved X-ray Diffuse Scattering (XDS), small differences in signal intensity are the starting point for analysis. Fluctuations in the total detected signal remain in the differences under investigation, obfuscating the signal. To correct such artefacts, Singular Value Decomposition (SVD) can be used to identify and characterize the observed detector fluctuations and assist in assigning some of them to variations in physical parameters such as X-ray energy and X-ray intensity. This paper presents a methodology for robustly identifying, separating and correcting fluctuations on area detectors based on XFEL beam characteristics, to enable the study of temporally resolved solution state chemistry on the femtosecond timescale.

Disentangling detector data in XFEL studies of temporally resolved solution state chemistry

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Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, SLAC National Accelerator Laboratory
Authors: Brandt van Driel, T. (Intern), Kjær, K. S. (Intern), Biasin, E. (Intern), Haldrup, K. (Intern), Lemke, H. T. (Ekstern), Nielsen, M. M. (Intern)
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Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.07 SJR 1.524 SNIP 0.903
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.489 SNIP 1.042 CiteScore 3.54
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.732 SNIP 1.274 CiteScore 3.79
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.645 SNIP 1.149 CiteScore 3.65
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.751 SNIP 0.938 CiteScore 3.24
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Scopus rating (2011): SJR 1.93 SNIP 1.232 CiteScore 3.92
ISI indexed (2011): ISI indexed no
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.755 SNIP 1.231
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.85 SNIP 1.168
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.819 SNIP 1.299
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.914 SNIP 1.315
Scopus rating (2006): SJR 1.548 SNIP 1.268
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Scopus rating (2005): SJR 1.655 SNIP 1.167
Scopus rating (2004): SJR 1.251 SNIP 1.093
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.231 SNIP 1.013
Scopus rating (2002): SJR 1.508 SNIP 1.033
Scopus rating (2001): SJR 1.783 SNIP 0.967
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**Doppler tomography in fusion plasmas and astrophysics**

Doppler tomography is a well-known method in astrophysics to image the accretion flow, often in the shape of thin discs, in compact binary stars. As accretion discs rotate, all emitted line radiation is Doppler-shifted. In fast-ion Dα (FIDA) spectroscopy measurements in magnetically confined plasma, the Dα-photons are likewise Doppler-shifted ultimately due to gyration of the fast ions. In either case, spectra of Doppler-shifted line emission are sensitive to the velocity distribution of the emitters. Astrophysical Doppler tomography has lead to images of accretion discs of binaries revealing bright spots, spiral structures and flow patterns. Fusion plasma Doppler tomography has led to an image of the fast-ion velocity distribution function in the tokamak ASDEX Upgrade. This image matched numerical simulations very well. Here we discuss achievements of the Doppler tomography approach, its promise and limits, analogies and differences in astrophysical and fusion plasma Doppler tomography and what can be learned by comparison of these applications.
In a thought-provoking paper, Couder and Fort [Phys. Rev. Lett. 97, 154101 (2006)] describe a version of the famous double-slit experiment performed with droplets bouncing on a vertically vibrated fluid surface. In the experiment, an interference pattern in the single-particle statistics is found even though it is possible to determine unambiguously which slit the walking droplet passes. Here we argue, however, that the single-particle statistics in such an experiment will be fundamentally different from the single-particle statistics of quantum mechanics. Quantum mechanical interference takes place between different classical paths with precise amplitude and phase relations. In the double-slit experiment with walking droplets, these relations are lost since one of the paths is singled out by the droplet. To support our conclusions, we have carried out our own double-slit experiment, and our results, in particular the long and variable slit passage times of the droplets, cast strong doubt on the feasibility of the interference claimed by Couder and Fort. To understand theoretically the limitations of wave-driven particle systems as analogs to quantum mechanics, we introduce a Schro"dinger equation with a source term originating from a localized particle that generates a wave while being simultaneously guided by it. We show that the ensuing particle-wave dynamics can capture some characteristics of quantum mechanics such as orbital quantization. However, the particle-wave dynamics can not reproduce quantum mechanics in general, and we show that the single-particle statistics for our model in a double-slit experiment with an additional splitter plate differs qualitatively from that of quantum mechanics.
Dual sightline measurements of MeV range deuterons with neutron and gamma-ray spectroscopy at JET

Observations made in a JET experiment aimed at accelerating deuterons to the MeV range by third harmonic radio-frequency (RF) heating coupled into a deuterium beam are reported. Measurements are based on a set of advanced neutron and gamma-ray spectrometers that, for the first time, observe the plasma simultaneously along vertical and oblique lines of sight. Parameters of the fast ion energy distribution, such as the high energy cut-off of the deuteron distribution function and the RF coupling constant, are determined from data within a uniform analysis framework for neutron and gamma-ray spectroscopy based on a one-dimensional model and by a consistency check among the individual measurement techniques. A systematic difference is seen between the two lines of sight and is interpreted to originate from the sensitivity of the oblique detectors to the pitch-angle structure of the distribution around the resonance, which is not correctly portrayed within the adopted one-dimensional model. A framework to calculate neutron and gamma-ray emission from a spatially resolved, two-dimensional deuteron distribution specified by energy/pitch is thus developed and used for a first comparison with predictions from ab initio models of RF heating at multiple harmonics.

The results presented in this paper are of relevance for the development of advanced diagnostic techniques for MeV range ions in high performance fusion plasmas, with applications to the experimental validation of RF heating codes and, more generally, to studies of the energy distribution of ions in the MeV range in high performance deuterium and deuterium-tritium plasmas.

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Web of Science (2015): Indexed yes
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ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
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Dynamic Behavior of CuZn Nanoparticles under Oxidizing and Reducing Conditions

The oxidation and reduction of CuZn nanoparticles was studied using X-ray photoelectron spectroscopy (XPS) and in situ transmission electron microscopy (TEM). CuZn nanoparticles with a narrow size distribution were produced with a gas-aggregation cluster source in conjunction with mass-filtration. A direct comparison between the spatially averaged XPS information and the local TEM observations was thus made possible. Upon oxidation in O₂, the as-deposited metal clusters transform into a polycrystalline cluster consisting of separate CuO and ZnO nanocrystals. Specifically, the CuO is observed to segregate to the cluster surface and partially cover the ZnO nanocrystals. Upon subsequent reduction in H₂, the CuO converts into metallic Cu with ZnO nanocrystal covering their surface. In addition, a small amount of metallic Zn is detected suggesting that ZnO is reduced. It is likely that Zn species can migrate to the Cu surface forming a Cu–Zn surface alloy. The oxidation and reduction dynamics of the CuZn nanoparticles is of great importance to industrial methanol synthesis for which the direct interaction of Cu and ZnO nanocrystals synergistically boosts the catalytic activity. Thus, the present results demonstrate a new model approach that should be generally applicable to address metal–support interactions in coprecipitated catalysts and multicomponent nanomaterials.
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Scopus rating (2001): SJR 1.783 SNIP 0.967
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Web of Science (2000): Indexed yes
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Effect of maghemization on the magnetic properties of nonstoichiometric pseudo-single-domain magnetite particles

The effect of maghemization on the magnetic properties of magnetite (Fe3O4) grains in the pseudo-single-domain (PSD) size range is investigated as a function of annealing temperature. X-ray diffraction and transmission electron microscopy confirm the precursor grains as Fe3O4 ranging from 150 to 250 nm in diameter, whilst Mössbauer spectrometry suggests the grains are initially near-stoichiometric. The Fe3O4 grains are heated to increasing reaction temperatures of 120–220°C to investigate their oxidation to maghemite (γ-Fe2O3). High-angle annular dark field imaging and localized electron-energy loss spectroscopy reveal slightly oxidized Fe3O4 grains, heated to 140°C, exhibit higher oxygen content at the surface. Off-axis electron holography allows for construction of magnetic induction maps of individual Fe3O4 and γ-Fe2O3 grains, revealing their PSD (vortex) nature, which is supported by magnetic hysteresis measurements, including first-order reversal curve analysis. The coercivity of the grains is shown to increase with reaction temperature up to 180°C, but subsequently decreases after heating above 200°C; this magnetic behavior is attributed to the growth of a γ-Fe2O3 shell with magnetic properties distinct from the Fe3O4 core. It is suggested there is exchange coupling between these separate components that results in a vortex state with reduced vorticity. Once fully oxidized to γ-Fe2O3, the domain states revert back to vortices with slightly reduced coercivity. It is argued that due to a core/shell coupling mechanism during maghemization, the directional magnetic information will still be correct; however, the intensity information will not be retained.

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Effect of maghemization on the magnetic properties of pseudo-single-domain magnetite particles

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Web of Science (2015): Indexed yes
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Scopus rating (2014): SJR 2.153 SNIP 1.226 CiteScore 3.01
Web of Science (2014): Indexed yes
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Scopus rating (2013): SJR 2.551 SNIP 1.209 CiteScore 3.12
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.77 SNIP 1.384 CiteScore 3.22
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 3.042 SNIP 1.244 CiteScore 3.05
ISI indexed (2011): ISI indexed yes
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BFI (2010): BFI-level 1
Scopus rating (2010): SJR 2.844 SNIP 1.308
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Scopus rating (2008): SJR 2.859 SNIP 1.154
Scopus rating (2007): SJR 2.541 SNIP 1.116
Scopus rating (2006): SJR 2.604 SNIP 1.304
Scopus rating (2005): SJR 2.643 SNIP 1.027
Scopus rating (2004): SJR 2.266 SNIP 1.124
Scopus rating (2003): SJR 2.716 SNIP 1.466
Scopus rating (2002): SJR 4.575 SNIP 1.481
Scopus rating (2001): SJR 1.555 SNIP 0.625
Original language: English

Effect of maghemization on the magnetic properties of pseudo-single-domain magnetite particles
Electron Injection from Copper Diimine Sensitizers into TiO₂: Structural Effects and Their Implications for Solar Energy Conversion Devices

Copper(I) diimine complexes have emerged as low cost replacements for ruthenium complexes as light sensitizers and electron donors, but their shorter metal-to-ligand-charge-transfer (MLCT) states lifetimes and lability of transient Cu(II) species impede their intended functions. Two carboxylated Cu(I) bis-2,9-diphenylphenanthroline (dpp) complexes [Cu(I)(dpp-O(CH₂CH₂O)₅)(dpp-(COOH)₂)]⁺ and [Cu(I)(dpp-O(CH₂CH₂O)₅)(dpp-(Φ-COOH)₂)]⁺ (Φ = tolyl) with different linker lengths were synthesized in which the MLCT-state solvent quenching pathways are effectively blocked, the lifetime of the singlet MLCT state is prolonged, and the transient Cu(II) ligands are stabilized. Aiming at understanding the mechanisms of structural influence to the interfacial charge transfer in the dye-sensitized solar cell mimics, electronic and geometric structures as well as dynamics for the MLCT state of these complexes and their hybrid with TiO₂ nanoparticles were investigated using optical transient spectroscopy, X-ray transient absorption spectroscopy, time-dependent density functional theory, and quantum dynamics simulations. The combined results show that these complexes exhibit strong absorption throughout the visible spectrum due to the severely flattened ground state, and a long-lived charge-separated Cu(II) has been achieved via ultrafast electron injection (<300 fs) from the 1MLCT state into TiO₂ nanoparticles. The results also indicate that the TiO₂-phen distance in these systems does not have significant effect on the efficiency of the interfacial electron-transfer process. The mechanisms for electron transfer in these systems are discussed and used to develop new strategies in optimizing copper(I) diimine complexes in solar energy conversion devices.

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Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Northwestern University, North Carolina State University, Korea Advanced Institute of Science & Technology, Argonne National Laboratory
Authors: Mara, M. W. (Ekstern), Bowman, D. N. (Ekstern), Buyukcakir, O. (Ekstern), Shelby, M. L. (Ekstern), Haldrup, K. (Intern), Huang, J. (Ekstern), Harpham, M. R. (Ekstern), Stickrath, A. B. (Ekstern), Zhang, X. (Ekstern), Stoddart, J. F. (Ekstern), Coskun, A. (Ekstern), Jakubikova, E. (Ekstern), Chen, L. X. (Ekstern)
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Scopus rating (2016): CiteScore 13.18 SJR 7.492 SNIP 2.596
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 6.775 SNIP 2.63 CiteScore 12.81
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 6.294 SNIP 2.587 CiteScore 11.92
Electron transport in molecular junctions

This thesis addresses the electron transport in molecular junctions, focusing on the energy level alignment and correlation effects. Various levels of theory have been applied to study the structural and electronic effects in different molecular junctions, starting from the single particle density functional theory (DFT) description over the semi-empirical DFT+Σ, to the sophisticated fully self-consistent GW approach. We find that in order to obtain a quantitative description of the conductance and the thermopower, it is necessary to go beyond the single particle description.

The effect of side groups on the benzene-diamine (BDA) molecule has furthermore been studied and it is found that the correct energy level alignment for the BDA molecule in Au contacts is only captured by the GW approach. Consequently, the GW approach provides an accurate description for the conductance change resulting from the side groups. The failure of the DFT based description is due to the strong energy level pinning when the BDA molecule is in contact with Au contacts.
The effect of contact geometries on the conductance and the thermopower has also been addressed. It is found that both GW and the DFT+\Sigma with a certain image charge position are in quantitative agreement with the experiments, while pure DFT is not. This is the consequence of the accurate energy level alignment, where the DFT+\Sigma method corrects the self-interaction error in the standard DFT functional and uses a static image charge model to include the image charge effect on the energy level renormalization.

Additionally, the gating of the 4,4'-bipyridine (44BP) molecule contacted to either Ni or Au electrodes has been investigated. Here it is found that the gating mechanism is conceptually different between two cases. In the case of Ni contacts where the lowest unoccupied molecular level (LUMO) of the 44BP molecule hybridizes strongly with Ni 3d orbitals, the gating is auxiliary by the so-called spinterface.

Finally, the correlation effect of the image charge beyond the energy level renormalization has been studied. It is shown that the finite response time of the electrodes to form image charge can suppress the conductance by a factor of 2. This correlation effect is only captured in the GW approach.

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**General information**

State: Published
Organisations: Department of Physics
Authors: Jin, C. (Intern), Thygesen, K. S. (Intern)
Number of pages: 111
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**Publication information**

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Main Research Area: Technical/natural sciences
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**Elliptic annular Josephson tunnel junctions in an external magnetic field: the statics:** Paper

We have investigated the static properties of one-dimensional planar Josephson tunnel junctions (JTJs) in the most general case of elliptic annuli. We have analyzed the dependence of the critical current in the presence of an external magnetic field applied either in the junction plane or in the perpendicular direction. We report a detailed study of both short and long elliptic annular junctions having different eccentricities. For junctions having a normalized perimeter less than one the threshold curves are derived and computed even in the case with one trapped Josephson vortex. For longer junctions a numerical analysis is carried out after the derivation of the appropriate perturbed sine-Gordon equation. For a given applied field we find that a number of different phase profiles exist which differ according to the number of fluxon-antifluxon pairs. We demonstrate that in samples made by specularly symmetric electrodes a transverse magnetic field is equivalent to an in-plane field applied in the direction of the current flow. Varying the ellipse eccentricity we reproduce all known results for linear and ring-shaped JTJs. Experimental data on high-quality Nb/Al-AlOx/Nb elliptic annular junctions support the theoretical analysis provided self-field effects are taken into account.

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**General information**

State: Published
Organisations: Department of Physics, Institute of Applied Sciences and Intelligent Systems 'E. Caianello'
Authors: Monaco, R. (Ekstern), Granata, C. (Ekstern), Vettoliere, A. (Ekstern), Mygind, J. (Intern)
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Scopus rating (2017): SNIP 1.426 SJR 1.036 CiteScore 2.63
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Enhanced ethanol production by removal of cutin and epicuticular waxes of wheat straw by plasma assisted pretreatment

The removal of cutin and epicuticular waxes of wheat straw by PAP (plasma assisted pretreatment) was investigated. Wax removal was observed by Attenuated Total Reflectance-Fourier Transform Infrared (ATR-FTIR) as chemical change on the surface of most intensively pretreated samples as well as with Scanning Electron Microscopy (SEM) imaging. Compounds resulting from wax degradation were analyzed in the washing water of PAP wheat straw. The wax removal enhanced enzymatic hydrolysis yield and, consequently, the efficiency of wheat straw conversion into ethanol. In total, PAP increased the conversion rate of the raw material carbohydrate content up to 67%, compared to untreated raw material.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, Department of Physics, Plasma Physics and Fusion Energy, Geological Survey of Denmark and Greenland, Frederiksberg High School, University of Copenhagen, Danish Technological Institute
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BFI (2017): BFI-level 2
Scopus rating (2017): SNIP 1.436 SJR 1.235 CiteScore 4
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.71 SJR 1.198 SNIP 1.385
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.51 SNIP 1.596 CiteScore 4.03
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.865 SNIP 1.964 CiteScore 4.36
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.666 SNIP 1.811 CiteScore 4.42
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Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.516 SNIP 1.754 CiteScore 3.66
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.759 SNIP 2.296 CiteScore 4.74
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.914 SNIP 2.251
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.728 SNIP 2.183
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Bioethanol, Enzymatic hydrolysis, Plasma assisted pretreatment, Simultaneous saccharification and fermentation, Wax removal, Fermentation

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Erratum: In Situ Studies of Fe$^{4+}$ Stability in $\beta$-Li$_3$Fe$_2$(PO$_4$)$_3$ Cathodes for Li Ion Batteries

General information
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Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, Department of Physics, Neutrons and X-rays for Materials Physics, Applied Electrochemistry, Fundamental Electrochemistry
Authors: Christiansen, A. S. (Intern), Johnsen, R. E. (Intern), Norby, P. (Intern), Frandsen, C. (Intern), Mørup, S. (Intern), Jensen, S. H. (Intern), Kammer Hansen, K. (Intern), Holtappels, P. (Intern)
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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
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Scopus rating (2014): SJR 1.213 SNIP 1.25 CiteScore 3.36
Excitons in van der Waals heterostructures: The important role of dielectric screening

The existence of strongly bound excitons is one of the hallmarks of the newly discovered atomically thin semiconductors. While it is understood that the large binding energy is mainly due to the weak dielectric screening in two dimensions, a systematic investigation of the role of screening on two-dimensional (2D) excitons is still lacking. Here we provide a critical assessment of a widely used 2D hydrogenic exciton model, which assumes a dielectric function of the form $\epsilon(q) = 1 + 2\pi\alpha q$, and we develop a quasi-2D model with a much broader applicability. Within the quasi-2D picture, electrons and holes are described as in-plane point charges with a finite extension in the perpendicular direction, and their interaction is screened by a dielectric function with a nonlinear $q$ dependence which is computed ab initio. The screened interaction is used in a generalized Mott-Wannier model to calculate exciton binding energies in both isolated and supported 2D materials. For isolated 2D materials, the quasi-2D treatment yields results almost identical to those of the strict 2D model, and both are in good agreement with ab initio many-body calculations. On the other hand, for more complex structures such as supported layers or layers embedded in a van der Waals heterostructure, the size of the
exciton in reciprocal space extends well beyond the linear regime of the dielectric function, and a quasi-2D description has to replace the 2D one. Our methodology has the merit of providing a seamless connection between the strict 2D limit of isolated monolayer materials and the more bulk-like screening characteristics of supported 2D materials or van der Waals heterostructures.

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Authors: Latini, S. (Intern), Olsen, T. (Intern), Thygesen, K. S. (Intern)
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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
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Scopus rating (2011): SJR 3.326 SNIP 1.423 CiteScore 3.61
ISI indexed (2011): ISI indexed yes
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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
Planar Hall effect magnetic field sensors with ring and diamond shaped geometries are experimentally compared with respect to their magnetic field sensitivity and total signal variation. Theoretically, diamond shaped sensors are predicted to be 41% more sensitive than corresponding ring shaped sensors for negligible shape anisotropy. To experimentally validate this, we have fabricated both sensor geometries in the exchange-biased stack Ni80Fe20(tFM)/Cu(tCu)/Mn80Ir20(10 nm) with tFM ¼ 10, 20, and 30 nm and tCu ¼ 0, 0.3, and 0.6 nm. Sensors from each stack were characterized by external magnetic field sweeps, which were analyzed in terms of a single domain model. The total signal variation of the diamond sensors was generally found to be about 40% higher than that for the ring sensors in agreement with theoretical predictions. However, for the low-field sensitivity, the corresponding improvement varied from 0% to 35% where the largest improvement was observed for sensor stacks with comparatively strong exchange bias. This is explained by the ring sensors being less affected by shape anisotropy than the diamond sensors. To study the effect of shape anisotropy, we also characterized sensors that were surrounded by the magnetic stack with a small gap of 3 μm. These sensors were found to be less affected by shape anisotropy and thus showed higher low-field sensitivities.
Extraction of light from a quantum emitter by tailoring the photonic environment

Since the discovery of quantum mechanics it has been a physicists dream to test and exploit the fantastic prediction of entanglement. Applications based on entanglement are quantum key distribution and quantum computing which can exploit ying quantum bits based on single photons. To deterministically create this type of quantum bits single photons on demand are essential. This thesis presents the work on controlling the photonic environment of a quantum emitter in order to efficiently extract photons.

We demonstrate increased photon collection efficiencies from single nitrogen vacancy (NV) centers by a factor of up to 1.76 when approaching it with a plane silver mirror made on an optical fiber facet. However, using this method we also
show that the non-radiative decay rate of NV centers can be highly dependent on the excitation power, which makes this method a poor broadband approach for obtaining information on the photonic decay rate of the NV center. By further spectrally resolving emission from these systems we observe clear modulations which carry information related to the photonic decay rate where the quantum efficiency can be deduced from.

We carry out three experiments where coupling NV centers to the highly confined mode fields of silver nano-wires (SNWs) are exploited. First, we demonstrate routing of single plasmons fed by a single NV center. Controlled routing is shown by facilitating different beamsplitter configurations where the routing itself is performed on a length scale less than 2 µm. We then measure the coupling between an NV center ensemble and single SNWs through 2-dimensional imaging of the NV center lifetime which outlines the SNW profiles confirmed by atomic force microscopy (AFM). Finally, an attempt to couple a single SNW to NV centers in a micro-fabricated diamond nano-pillar is presented.

The final part of the thesis address experiments on coupling colloidal quantum dots (CQDs) to the gap mode of two Si3N4 waveguides (DSNWs). We demonstrate evanescent-field coupling between spin-coated CQDs and the waveguide. However we are unable to deduce the coupling-related modification of the CQD lifetime due to apparent density dependent CQD interactions which dominate the lifetime distribution. We circumvent this by instead attaching CQDs to an AFM cantilever and scanning this across the DSNWs. By doing this, we obtain a 2-dimensional lifetime map showing an AFM-confirmed outline of the DSNW through the spatially-dependant lifetime variations.

General information
State: Published
Organisations: Department of Photonics Engineering, Fiber Sensors and Supercontinuum Generation, Department of Physics, Quantum Physics and Information Technology
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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-xSrMnO3 (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.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Electrofunctional materials, Department of Physics, University of Twente, University of British Columbia, University of Antwerp, University of Saskatchewan, Weizmann Institute of Science, University of Copenhagen
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Main Research Area: Technical/natural sciences

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Journal: Nature Materials
Far scrape-off layer particle and heat fluxes in high density: High power scenarios
The far scrape-off layer transport is studied in ASDEX Upgrade H-mode discharges with high divertor neutral density $N_{0,\text{div}}$, high power across the separatrix $P_{\text{sep}}$ and nitrogen seeding to control the divertor temperature. Such conditions are expected for ITER but usually not investigated in terms of turbulent SOL transport. At high $N_{0,\text{div}}$ and $P_{\text{sep}}$ the H-mode discharges enter a regime of high cross-field particle and power transport in the SOL which is accompanied by a significant change of the turbulence characteristic analogous to the transition from conductive to convective transport in L-mode. Parallel particle and power flux densities of several $10^{23} \text{ m}^{-2} \text{ s}^{-1}$ and 10 MW m$^{-2}$ have been detected about $\sim 40$ to 45 mm outside the separatrix mapped to the outer mid-plane. The particle flux fall-off length reached up to 45 mm. This paper presents for the first time an empirical condition to enter the high transport regime in H-mode and the relation of this regime to changes in the filamentary transport.

Fast & scalable pattern transfer via block copolymer nanolithography
A fully scalable and efficient pattern transfer process based on block copolymer (BCP) self-assembling directly on various substrates is demonstrated. PS-rich and PDMS-rich poly(styrene-b-dimethylsiloxane) (PS-b-PDMS) copolymers are used to give monolayer sphere morphology after spin-casting of solutions with selective solvents relative to the majority block. The pattern is directly formed during spin-casting at room temperature, which takes less than 20 seconds, without any preliminary surface treatment of the substrate and without any subsequent annealing. The self-assembled BCPs are transformed into hard lithography masks by oxidation of PDMS in oxygen plasma. The hard masks are then used to fabricate full wafer scale arrays of nano-pillars and nano-wells on various substrates, including polymers and silicon. The demonstrated BCP nano-lithography process opens up numerous applications not relying on long range lateral order, including fabrication of substrates for catalysis, solar cells, sensors, ultrafiltration membranes and templating of semiconductors or metals.

Far scrape-off layer particle and heat fluxes in high density: High power scenarios
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Fast and sensitive method for detecting volatile species in liquids

This paper presents a novel apparatus for extracting volatile species from liquids using a “sniffer-chip.” By ultrafast transfer of the volatile species through a perforated and hydrophobic membrane into an inert carrier gas stream, the sniffer-chip is able to transport the species directly to a mass spectrometer through a narrow capillary without the use of differential pumping. This method inherits features from differential electrochemical mass spectrometry (DEMS) and membrane inlet mass spectrometry (MIMS), but brings the best of both worlds, i.e., the fast time-response of a DEMS system and the high sensitivity of a MIMS system. In this paper, the concept of the sniffer-chip is thoroughly explained and it is shown how it can be used to quantify hydrogen and oxygen evolution on a polycrystalline platinum thin film in situ at absolute faradaic currents down to ~30 nA. To benchmark the capabilities of this method, a CO-stripping experiment is performed on a polycrystalline platinum thin film, illustrating how the sniffer-chip system is capable of making a quantitative in situ measurement of <1 % of a monolayer of surface adsorbed CO being electrochemically stripped off an electrode at a potential scan-rate of 50 mV s⁻¹.

General information
State: Published
Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics, Department of Micro- and Nanotechnology, Silicon Microtechnology
Authors: Trimarco, D. B. (Intern), Pedersen, T. (Intern), Hansen, O. (Intern), Chorkendorff, I. (Intern), Vesborg, P. C. K. (Intern)
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BFI (2018): BFI-level 1
Fast Characterization of Moving Samples with Nano-Textured Surfaces

Characterization of structures using conventional optical microscopy is restricted by the diffraction limit. Techniques like atomic force and scanning electron microscopy can investigate smaller structures but are very time consuming. We show that using scatterometry, a technique based on optical diffraction, integrated into a commercial light microscope we can characterize nano-textured surfaces in a few milliseconds. The adapted microscope has two detectors, a CCD camera used to easily find an area of interest and a spectrometer for the measurements. We demonstrate that the microscope has a resolution in the nanometer range for the topographic parameters: height, width, and sidewall angle of a periodic grating, also in an environment with many vibrations, such as a production facility with heavy equipment.

Fast-ion transport and neutral beam current drive in ASDEX upgrade

The neutral beam current drive efficiency has been investigated in the ASDEX Upgrade tokamak by replacing on-axis neutral beams with tangential off-axis beams. A clear modification of the radial fast-ion profiles is observed with a fast-ion D-alpha diagnostic that measures centrally peaked profiles during on-axis injection and outwards shifted profiles during off-axis injection. Due to this change of the fast-ion population, a clear modification of the plasma current profile is predicted but not observed by a motional Stark effect diagnostic. The fast-ion transport caused by MHD activity has been studied in low collisionality discharges that exhibit strong (1, 1) modes. In particular due to sawtooth crashes, significant radial redistribution of co-rotating fast-ions is observed which can very well be described by the Kadomtsev model. In addition, first tomographic reconstructions of the central 2D fastion velocity space in the presence of sawtooth crashes allow the investigation of the pitch dependence of the mode-imposed redistribution: a stronger redistribution of mainly co-rotating fast ions is observed than of those with smaller pitch values.
While investigating uniformity of magnetic tunnel junction (MTJ) stacks we find experimentally and analytically that variation in the resistance area product (RA) is more important to monitor as compared to the tunnel magnetoresistance (TMR), which is less sensitive to MTJ variability. The standard Current In-Plane Tunneling (CIPT) method measures both RA and TMR, but the usefulness for uniformity mapping, e.g. for tool optimization, is limited by excessive measurement time. Thus, we develop and demonstrate a fast complementary static magnetic field method focused only on measurement of RA. We compare the static field method to the standard CIPT method and find perfect agreement between the extracted RA values and measurement repeatability while the static field method is several times faster. The static field CIPT method is demonstrated for 200 mm wafer mapping showing radial as well as asymmetrical variations related to the MTJ deposition conditions.
Fiber-Based, Injection-Molded Optofluidic Systems: Improvements in Assembly and Applications

We present a method to fabricate polymer optofluidic systems by means of injection molding that allow the insertion of standard optical fibers. The chip fabrication and assembly methods produce large numbers of robust optofluidic systems that can be easily assembled and disposed of, yet allow precise optical alignment and improve delivery of optical power. Using a multi-level chip fabrication process, complex channel designs with extremely vertical sidewalls, and dimensions that range from few tens of nanometers to hundreds of microns can be obtained. The technology has been used to align optical fibers in a quick and precise manner, with a lateral alignment accuracy of 2.7 ± 1.8 μm. We report the production, assembly methods, and the characterization of the resulting injection-molded chips for Lab-on-Chip (LoC) applications. We demonstrate the versatility of this technology by carrying out two types of experiments that benefit from the improved optical system: optical stretching of red blood cells (RBCs) and Raman spectroscopy of a solution loaded into a hollow core fiber. The advantages offered by the presented technology are intended to encourage the use of LoC technology for commercialization and educational purposes.
Field-induced interplanar magnetic correlations in the high-temperature superconductor La_{1.88}Sr_{0.12}CuO_4

We present neutron-scattering studies of the interplanar magnetic correlations in the high-temperature superconductor La_{1.88}Sr_{0.12}CuO_4 (T_c = 27 K). The correlations are studied both in a magnetic field applied perpendicular to the CuO2 planes, and in zero field under different cooling conditions. We find that the effect of the magnetic field is to increase the magnetic scattering signal at all values of the out-of-plane wave vector L, indicating an overall increase of the magnetic moments. In addition, weak correlations between the copper oxide planes develop in the presence of a magnetic field. This effect is not taken into account in previous reports on the field effect of magnetic scattering, since usually only L=0 is probed. Interestingly, the results of quench-cooling the sample are similar to those obtained by applying a magnetic field. Finally, a small variation of the incommensurate peak position as a function of L provides evidence that the incommensurate signal is twinned with the magnetic scattering from the dominant and subdominant structural twin displaying peaks at even and odd values of L, respectively, in our crystal.
First operations with the new Collective Thomson Scattering diagnostic on the Frascati Tokamak Upgrade device

Anomalous emissions were found over the last few years in spectra of Collective Thomson Scattering (CTS) diagnostics in tokamak devices such as TEXTOR, ASDEX and FTU, in addition to real CTS signals. The signal frequency, down-shifted with respect to the probing one, suggested a possible origin in Parametric Decay Instability (PDI) processes correlated with the presence of magnetic islands and occurring for pumping wave power levels well below the threshold predicted by conventional models. A threshold below or close to the Electron Cyclotron Resonance Heating (ECRH) power levels could limit, under certain circumstances, the use of the ECRH in fusion devices. An accurate characterization of the conditions for the occurrence of this phenomenon and of its consequences is thus of primary importance. Exploiting the front-steering configuration available with the real-time launcher, the implementation of a new CTS setup now allows studying these anomalous emission phenomena in FTU under conditions of density and wave injection geometry that are more similar to those envisaged for CTS in ITER. The upgrades of the diagnostic are presented as well as a few preliminary spectra detected with the new system during the very first operations in 2014.

General information
State: Published
Authors: Bin, W. (Ekstern), Bruschi, A. (Ekstern), D'Arcangelo, O. (Ekstern), Castaldo, C. (Ekstern), Angeli, M. D. (Ekstern), Figini, L. (Ekstern), Galperti, C. (Ekstern), Garavaglia, S. (Ekstern), Granucci, G. (Ekstern), Grosso, G. (Ekstern), Korsholm, S. B. (Intern), Lontano, M. (Ekstern), Melli, L. (Ekstern), Moro, A. (Ekstern), Nardone, A. (Ekstern), Nielsen, S. K. (Intern), Rasmussen, J. (Intern), Simonetto, A. (Ekstern), Pedersen, M. S. (Intern), Tartari, U. (Ekstern)
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BFI (2012): BFI-level 1
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First principle numerical simulations of the SOL in ASDEX Upgrade

General information
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Organisations: Department of Physics, Plasma Physics and Fusion Energy, University of Cyprus, Institute for Magnetic Fusion Research, Max Planck Institute, Instituto de Plasmas e Fusão Nuclear, VTT - Technical Research Centre of Finland, Max-Planck-Institut fur Plasmaphysik, Ecole Polytechnique Federale de Lausanne (EPFL), University of Innsbruck
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First Principle simulations of electrochemical interfaces - a DFT study
In this thesis, I have looked beyond the computational hydrogen electrode (CHE) model, and focused on the first principle simulations which treats the electrode-electrolyte interfaces explicitly. Since obtaining a realistic electrode-electrolyte interface was difficult, I aimed to address various challenges regarding first principle electrochemical interface modeling in order to bridge the gap between the model interface used in simulations and real catalyst at operating conditions. Atomic scale insight for the processes and reactions that occur at the electrochemical interface presents a challenge to both, the experimentalists, and the theorists. Energetics of charge transfer reactions over the electrochemical interface, determines, to a great extent, the efficiency of energy conversion. Therefore, gaining an atomic-level understanding of the interface, have utmost importance. Experimentalists measure macroscopic quantities, e.g., current versus voltage and have no direct information about the corresponding interfacial atomic structure. However, scanning tunneling microscope (STM) might be useful in disclosing information about the atomic structure, but it can not be performed in situ in aqueous electrolytes in order to reveal metal-water interfacial structure.
First principle calculations are useful in disclosing interfacial atomic structure, however, theorists, have other challenges to deal. Atomic scale modeling of the electrochemical interface, is still far from realistic. The real electrochemical interface is challenging to model because processes that take place over the interface are complicated. First principle methods have
limitations due to the various approximations in implementations and may sometimes lead to incorrect electronic structure at the electrochemical interface, which can result in an improper/ill-defined electrochemical interface. Considering the electronic structure of the interface, I have mentioned some of the pitfalls in modeling electrochemical interfaces, and I have also shown how to avoid these pitfalls. The electrode-electrolyte interface models constructed without care for electronic structure, could exhibit an unphysical charge transfer due to the DFT's notorious under-estimation of the HUMO-LUMO gap. For such systems, electrode potential cannot be tuned. I have shown that the HOMO-LUMO gap of the electrolyte have to straddle the Fermi level, in order for the whole system to qualify as a proper electrochemical interface.

I have also contributed to the model, which accounts for pH in the first principle electrode-electrolyte interface simulations. This is an important step forward, since electrochemical reaction rate and barrier for charge transfer can strongly depend on pH. I have shown that pH can have influence over the interface structure, and hence can influence the adsorbate free energies with direct hydrogen bonding or chemical interactions with the electrolyte dipole. Therefore, in order to study the reactions at constant electrochemical potential, pH has to be kept constant together with the chemical potential of protons and electrons. However, this was not the case for some of the calculations reported in the literature for constant electrochemical potential, where the calculations are not really done at constant electrochemical potential, as the chemical potential of proton (or pH) was not considered. However, in most of the cases, the effect of pH was negligible. We have applied this developed model to Pt(111)-water interface as an example, and constructed the corresponding Pourbaix diagram, which shows the effect of pH and potential on adsorbate coverage and interface structure. I have also investigated the pH effect on the electrochemical adsorption of hydrogen for Pt(100) and Pt(111) surfaces by applying the above model that account for pH in the simulations. As a consequence of negligible interaction between electrolyte and adsorbed hydrogen, I found that modeled electrochemical interface and pH have no influence over hydrogen adsorption energy. In fact, hydrogen adsorption is well defined by considering just CHE model. However, barrier for charge transfer, can depend on the pH, as pH can influence the water structure at the interface. I have also discussed a scenario, where proton is more stable at the electrochemical interface, where the water layer is almost chemi-adsorbed at the surface. This is an interesting case as proton being stable in the Outer Helmholz Plane (OHP), significantly change the electrostatic potential in the double layer region. This might also have an impact over barrier for charge transfer considering hydrogen evolution reaction (HER). I have also calculated the pseudo-capacitances for hydrogen adsorption region for both surfaces, which agrees with experiments.

**General information**

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Organisations: Department of Physics

Authors: Ahmed, R. (Intern), Rossmeisl, J. (Intern)

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**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.

**General information**

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Organisations: Center for Atomic-scale Materials Design, Department of Physics, Department of Energy Conversion and Storage, Atomic scale modelling and materials

Authors: Tripkovic, V. (Intern), Hansen, H. A. (Intern), Rossmeisl, J. (Intern), Vegge, T. (Intern)

Pages: 11647-11657
First principles study of (Cd, Hg, In, Ti, Sn, Pb, As, Sb, Bi, Se) modified Pt(111), Pt(100) and Pt(211) electrodes as CO oxidation catalysts

CO oxidation is a prototype reaction for studying oxidation of small organic molecules. Certain adatom modified Pt electrodes have a large promotional effect on CO oxidation. However, the effect is often coverage dependent, and has a limited effect due to short lifetimes of the adatoms. The coverage dependence as a function of potential for ten different adatom species (Cd, Hg, In, Ti, Sn, Pb, As, Sb, Bi, Se) on bare and CO saturated Pt(111), Pt(100) and Pt(211) surfaces has been established by means of Density Functional Theory calculations. Most of the adatoms are very stable under standard conditions and remain anchored to the surface until high potentials in supporting electrolytes. The stability is contingent on the electrode roughness and reduces in the following order: Pt(211) ≈ Pt(100) > Pt(111), except for Se adatoms, in which case the trend is reversed. The activity for CO oxidation, given by the OH formation potentials from water, is dependent on the oxophilicity of the adatoms, and is found to scale almost inversely with the adatom stability. In electrolyte solutions saturated with CO, the stability reduces to roughly half of that on bare Pt surfaces. Irrespective of the CO partial pressure, most of the adatoms are found to dissolve before they become oxidized. This has a detrimental impact on the reaction as high activities have been associated with oxidized adatoms moieties. As on Pt(100) is the only adatom electrode stable in a narrow potential range under standard conditions.
In the present study, on the basis of detailed density functional theory (DFT) calculations, and using Ni hydroxy(oxide) films on Pt(111) and Au(111) electrodes as model systems, we describe a detailed structural and electrocatalytic analysis of hydrogen evolution (HER) at three-phase boundaries under alkaline electrochemical conditions. We demonstrate that the structure and oxidation state of the films can be systematically tuned by changing the applied electrode potential and/or the nature of substrates. Structural features determined from the theoretical calculations provide a wealth of information that is inaccessible by purely experimental means, and these structures, in turn, strongly suggest that a bifunctional reaction mechanism for alkaline HER will be operative at the interface between the films, the metal substrates, and the surrounding aqueous medium. This bifunctionality produces important changes in the calculated barriers of key elementary reaction steps, including water activation and dissociation, as compared to traditional monofunctional Pt surfaces.
The successful identification of the structures of thin metal films and three-phase boundary catalysts is not only an important step towards accurate identification and prediction of a variety of oxide/electrode interfacial structure-properties relationships, but also provides the foundation for rational design and control of ‘targeted active phases’ at catalytic interfaces. The successful design of bifunctional electrocatalysts that exploit these structures, in turn, could ultimately lead to advances in the development of alkaline fuel cells.

**Forandringens vinde - Nye Teknologihistorier**

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State: Published
Organisations: Department of Physics
Authors: Zwisler, L. (Intern)
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Main Research Area: Technical/natural sciences

**Forces acting on a small particle in an acoustical field in a thermoviscous fluid**

We present a theoretical analysis of the acoustic radiation force on a single small spherical particle, either a thermoviscous fluid droplet or a thermoelastic solid particle, suspended in a viscous and heat-conducting fluid medium. Within the perturbation assumptions, our analysis places no restrictions on the length scales of the viscous and thermal boundary-layer thicknesses $\delta_s$ and $\delta_t$ relative to the particle radius $a$, but it assumes the particle to be small in comparison to the acoustic wavelength $\lambda$. This is the limit relevant to scattering of ultrasound waves from nanometer- and micrometer-sized particles. For particles of size comparable to or smaller than the boundary layers, the thermoviscous theory leads to profound consequences for the acoustic radiation force. Not only do we predict forces orders of magnitude larger than expected from ideal-fluid theory, but for certain relevant choices of materials, we also find a sign change in the acoustic radiation force on different-sized but otherwise identical particles. These findings lead to the concept of a particle-size-dependent acoustophoretic contrast factor, highly relevant to acoustic separation of microparticles in gases, as well as to handling of nanoparticles in lab-on-a-chip systems.

**General information**
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Organisations: Department of Physics, Biophysics and Fluids, Department of Micro- and Nanotechnology
Authors: Karlsen, J. T. (Intern), Bruus, H. (Intern)
Formation and transformation of a short range ordered iron carbonate precursor

Fe(II)-carbonates, such as siderite, form in environments where O₂ is scarce, e.g., during marine sediment diagenesis, corrosion and possibly CO₂ sequestration, but little is known about their formation pathways. We show that early precipitates from carbonate solutions containing 0.1M Fe(II) with varying pH produced broad peaks in X-ray diffraction and contained dominantly Fe and CO₃ when probed with X-ray photoelectron spectroscopy. Reduced pair distribution function (PDF) analysis shows only peaks corresponding to interatomic distances below 15Å, reflecting a material with no long range structural order. Moreover, PDF peak positions differ from those for known iron carbonates and hydroxides. Mössbauer spectra also deviate from those expected for known iron carbonates and suggest a less crystalline structure. These data show that a previously unidentified iron carbonate precursor phase formed. Its coherent scattering domains determined from PDF analysis are slightly larger than for amorphous calcium carbonate, suggesting that the precursor could be nanocrystalline. Replica exchange molecular dynamics simulations of Fe-carbonate polynuclear complexes yield PDF peak positions that agree well with those from experiments, offering the possibility that the material is a condensate of such complexes, assembled in a relatively unorganised fashion. If this is the case, the material could be nearly amorphous, rather than being composed of well defined nanocrystals. PDF measurements of samples ageing in solution coupled with refinement with the software PDFgui show that the material transforms to siderite or siderite/chukanovite mixtures within hours and that the transformation rate depends on pH. The identified Fe-carbonate precursor may potentially form during anaerobic corrosion or bacterial Fe reduction.
Fractional excitations in the square-lattice quantum antiferromagnet

Quantum magnets have occupied the fertile ground between many-body theory and low-temperature experiments on real materials since the early days of quantum mechanics. However, our understanding of even deceptively simple systems of interacting spin-1/2 particles is far from complete. The quantum square-lattice Heisenberg antiferromagnet, for example, exhibits a striking anomaly of hitherto unknown origin in its magnetic excitation spectrum. This quantum effect manifests itself for excitations propagating with the specific wavevector \((\pi, 0)\). We use polarized neutron spectroscopy to fully characterize the magnetic fluctuations in the metal-organic compound \(\text{Cu(DCOO)}_2\cdot 4\text{D}_2\text{O}\), a known realization of the quantum square-lattice Heisenberg antiferromagnet model. Our experiments reveal an isotropic excitation continuum at the anomaly, which we analyse theoretically using Gutzwiller-projected trial wavefunctions. The excitation continuum is accounted for by the existence of spatially extended pairs of fractional \(S=1/2\) quasiparticles, 2D analogues of 1D spinons. Away from the anomalous wavevector, these fractional excitations are bound and form conventional magnons. Our results establish the existence of fractional quasiparticles in the high-energy spectrum of a quasi-two-dimensional antiferromagnet, even in the absence of frustration.
Results based on virtual instrument models for the first high-flux, high-resolution, spallation based, backscattering spectrometer, BASIS are presented in this paper. These were verified using the Monte Carlo instrument simulation packages McStas and VITESS. Excellent agreement of the neutron count rate at the sample position between the virtual instrument simulation and experiments was found, in both time and energy distributions. This achievement was only possible after a new component for a bent single crystal analyser in McStas, using a Gaussian approximation, was developed. These findings are pivotal to the conceptual design of the next generation backscattering spectrometer, MIRACLES at the European Spallation Source.
Gamma-ray emission spectrum from thermonuclear fusion reactions without intrinsic broadening

First principle calculations of the gamma-ray energy spectrum arising from thermonuclear reactions without intrinsic broadening in fusion plasmas are presented, extending the theoretical framework needed to interpret measurements up to the accuracy level enabled by modern high resolution instruments. An analytical formula for the spectrum from Maxwellian plasmas, which extends to higher temperatures than the results previously available in the literature, has been derived and used to discuss the assumptions and limitations of earlier models. In case of radio-frequency injection, numerical results based on a Monte Carlo method are provided, focusing in particular on improved relations between the peak shift and width from the reaction and the temperature of protons accelerated by radio-frequency heating. The results presented in this paper significantly improve the accuracy of diagnostic information that can be extracted from the gamma-ray emission spectrum of fusion reactions without intrinsic broadening and are of relevance for applications to high performance fusion plasmas.
plasmas of present and next generation devices.

**General information**
- State: Published
- Organisations: Department of Physics, Plasma Physics and Fusion Energy, University of Milano Bicocca, Uppsala University, Consiglio Nazionale delle Ricerche
- Authors: Nocente, M. (Ekstern), Källne, J. (Ekstern), Salewski, M. (Intern), Tardocchi, M. (Ekstern), Gorini, G. (Ekstern)
- Number of pages: 11
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  - Web of Science (2017): Indexed yes
  - BFI (2016): BFI-level 1
  - Scopus rating (2016): CiteScore 1.62 SJR 1.284 SNIP 1.416
  - Web of Science (2016): Indexed yes
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  - Scopus rating (2015): SJR 1.51 SNIP 1.62 CiteScore 1.88
  - Web of Science (2015): Indexed yes
  - BFI (2014): BFI-level 1
  - Scopus rating (2014): SJR 1.907 SNIP 1.667 CiteScore 2.2
  - Web of Science (2014): Indexed yes
  - BFI (2013): BFI-level 1
  - Scopus rating (2013): SJR 1.366 SNIP 1.516 CiteScore 1.83
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  - Scopus rating (2012): SJR 1.441 SNIP 1.448 CiteScore 1.81
  - ISI indexed (2012): ISI indexed yes
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  - BFI (2011): BFI-level 1
  - Scopus rating (2011): SJR 2.043 SNIP 2.433 CiteScore 3.78
  - ISI indexed (2011): ISI indexed yes
  - Web of Science (2011): Indexed yes
  - BFI (2010): BFI-level 1
  - Scopus rating (2010): SJR 2.268 SNIP 1.927
  - Web of Science (2010): Indexed yes
  - BFI (2009): BFI-level 1
  - Scopus rating (2009): SJR 1.993 SNIP 2.441
  - Web of Science (2009): Indexed yes
  - BFI (2008): BFI-level 1
  - Scopus rating (2008): SJR 2.031 SNIP 1.736
  - Web of Science (2008): Indexed yes
  - Scopus rating (2007): SJR 2.005 SNIP 1.987
  - Web of Science (2007): Indexed yes
  - Scopus rating (2006): SJR 2.062 SNIP 1.937
  - Web of Science (2006): Indexed yes
Generalized balanced power diagrams for 3D representations of polycrystals

Characterizing the grain structure of polycrystalline material is an important task in material science. The present paper introduces the concept of generalized balanced power diagrams as a concise alternative to voxelated mappings. Here, each grain is represented by (measured approximations of) its centre of mass position, its volume and, if available, and by its second-order moments (in the non-equiaxed case). Such parameters may be obtained from 3D X-ray diffraction. As the exact global optimum of our model results from the solution of a suitable linear programme it can be computed quite efficiently. Based on verified real-world measurements, we show that from the few parameters per grain (3, respectively, 6 in 2D and 4, respectively, 10 in 3D) we obtain excellent representations of both equiaxed and non-equiaxed structures. Hence our approach seems to capture the physical principles governing the forming of such polycrystals in the underlying process quite well.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Technische Universität München, Universität der Bundeswehr München, Xnovo Technology ApS
Authors: Alpers, A. (Ekstern), Brieden, A. (Ekstern), Gritzmann, P. (Ekstern), Lyckegaard, A. (Ekstern), Poulsen, H. F. (Intern)
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BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.34 SJR 0.698 SNIP 0.708
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.883 SNIP 0.925 CiteScore 1.52
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 0.939 SNIP 1.073 CiteScore 1.56
Web of Science (2014): Indexed yes
Gold Nanoparticle-Based Sensors Activated by External Radio Frequency Fields

A novel molecular beacon (a nanomachine) is constructed that can be actuated by a radio frequency (RF) field. The nanomachine consists of the following elements arranged in molecular beacon configuration: a gold nanoparticle that acts both as quencher for fluorescence and a localized heat source; one reporter fluorochrome, and; a piece of DNA as a hinge and recognition sequence. When the nanomachines are irradiated with a 3 GHz RF field the fluorescence signal increases due to melting of the stem of the molecular beacon. A control experiment, performed using molecular beacons synthesized by substituting the gold nanoparticle by an organic quencher, shows no increase in fluorescence signal when exposed to the RF field. It may therefore be concluded that the increased fluorescence for the gold nanoparticle-conjugated nanomachines is not due to bulk heating of the solution, but is caused by the presence of the gold nanoparticles and their interaction with the RF field; however, existing models for heating of gold nanoparticles in a RF field are unable to explain the experimental results. Due to the biocompatibility of the construct and RF treatment, the nanomachines may possibly be used inside living cells. In a separate experiment a substantial increase in the dielectric losses can be detected in a RF waveguide setup coupled to a microfluidic channel when gold nanoparticles are added to a low RF loss liquid. This work sheds some light on RF heating of gold nanoparticles, which is a subject of significant controversy in the literature.

General information
State: Published
Organisations: Department of Micro- and Nanotechnology, Silicon Microtechnology, Fluidic Array Systems and Technology, Department of Electrical Engineering, Electromagnetic Systems, Center for Electron Nanoscopy, Polymer Microsystems for Cell Processing, Experimental Surface and Nanomaterials Physics
Graphene transfer on highly corrugated black silicon surface

General information
State: Published
Organisations: Department of Micro- and Nanotechnology, Silicon Microtechnology, Center for Nanostructured Graphene, Self-Organized Nanoporous Materials, Nanocarbon, Experimental Surface and Nanomaterials Physics
Authors: Plakhotnyuk, M. (Intern), Shvets, V. (Intern), Whelan, P. R. (Intern), Mackenzie, D. (Intern), Bøggild, P. (Intern), Hansen, O. (Intern)
Number of pages: 2
Publication date: 2015
Event: Abstract from 6th Symposium on Carbon and Related Nanomaterials, Copenhagen, Denmark.
Main Research Area: Technical/natural sciences
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Green preparation and spectroscopic characterization of plasmonic silver nanoparticles using fruits as reducing agents
Chemicals typically available in plants have the capability to reduce silver and gold salts and to create silver and gold nanoparticles. We report the preparation of silver nanoparticles with sizes between 10 and 300 nm from silver nitrate using fruit extract collected from pineapples and oranges as reducing agents. The evolvement of a characteristic surface plasmon extinction spectrum in the range of 420 nm to 480 nm indicates the formation of silver nanoparticles after mixing silver nitrate solution and fruit extract. Shifts in plasmon peaks over time indicate the growth of nanoparticles. Electron microscopy shows that the shapes of the nanoparticles are different depending on the fruit used for preparation.
The green preparation process results mainly in individual nanoparticles with a very poor tendency to form aggregates with narrow gaps even when aggregation is forced by the addition of NaCl. This explains only modest enhancement factors for near-infrared-excited surface enhanced Raman scattering.
In addition to the surface plasmon band, UV-visible absorption spectra show features in the UV range which indicates also the presence of small silver clusters, such as Ag42+. The increase of the plasmon absorption correlates with the decrease of absorption band in the UV. This confirms the evolution of silver nanoparticles from silver clusters.
The presence of various silver clusters on the surface of the “green” plasmonic silver nanoparticles is also supported by a strong multi-color luminesce signal emitted by the plasmonic particles during 473 nm excitation.

General information
State: Published
Organisations: Department of Micro- and Nanotechnology, Fluidic Array Systems and Technology, Department of Physics, Biophysics and Fluids, Technical University of Denmark
Authors: Hyllested, J. Æ. (Ekstern), Espina Palanco, M. (Intern), Hagen, N. (Ekstern), Mogensen, K. B. (Intern), Kneipp, K. (Intern)
Pages: 293-299
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Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.86 SJR 1.138 SNIP 1.026
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Gyrofluid potential vorticity equation and turbulent equipartion states: Paper

An equation governing potential vorticity in a magnetized plasmas is derived. The equation is analogous to Ertel’s theorem. In the long wave-length limit the potential vorticity equals the ratio of the gyro-frequency plus the E × B- and diamagnetic polarization densities to the particle density. The equation is relevant for transport barriers in magnetically confined plasmas because particle density, ion temperature and the radial electric field are mutually coupled through the potential vorticity. The potential vorticity equation is derived from an energy conserving, four-field, electrostatic, full-F gyrofluid model. It is shown that the gyrofluid model possesses two exact Lagrangian invariants. In systems where mixing uniformly distribute the Lagrangian invariants we derive the corresponding turbulent equipartion states. It is shown that the system is driven towards constant potential vorticity. Given particle density and magnetic field profiles we infer ion temperature and electric potential profiles from the derived turbulent equipartion states.
Heats of formation of solids with error estimation: The mBEEF functional with and without fitted reference energies

The need for prediction of accurate electronic binding energies has led to the development of different schemes for combining density functional calculations, typically at the level of the generalized gradient approximation (GGA), with experimental information. We analyze one such scheme by Stevanovic’ et al. [Phys. Rev. B85, 115104 (2012)PRBMDO1098-012110.1103/PhysRevB.85.115104] for predictions of compound enthalpies of formation using fitted elemental-phase reference energies. We show that different versions of GGA with or without +U and a meta-GGA (TPSS) lead to comparable accuracy after fitting the reference energies. Our results also show that the recently developed mBEEF, a Bayesian error estimation functional, gives comparable accuracy with the other functionals even without the fitting. The mBEEF functional furthermore supplies an ensemble estimate of the prediction errors in reasonable agreement with the actual errors. We also show that using the fitting scheme on the mBEEF ensemble leads to improved accuracy including realistic error estimation.

General information
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Organisations: Center for Atomic-scale Materials Design, Department of Physics
Authors: Pandey, M. (Intern), Jacobsen, K. W. (Intern)
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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
High-Jc \( \text{YBa}_2\text{Cu}_3\text{O}_{7-x}\)-Ag superconducting thin films synthesized through a fluorine-free MOD method

Obtaining a high critical current density (\( J_c \)) 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 \( J_c \) values in this research work. By reacting with propionic acid and ammonia, \( \text{AgNO}_3 \) 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 \( J_c \) of 4.6MA/cm² was obtained in a YBCO-Ag thin film with 10 wt% Ag.

General information
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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)
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Scopus rating (2017): CiteScore 3.55 SJR 1.068 SNIP 1.698
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
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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
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Scopus rating (2014): SJR 1.163 SNIP 2.083 CiteScore 3.16
Web of Science (2014): Indexed yes
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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
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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
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.139 SNIP 1.627
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.212 SNIP 1.745
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.22 SNIP 1.665
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.095 SNIP 1.633
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.055 SNIP 1.743
Scopus rating (2003): SJR 1.151 SNIP 1.496
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
Highly efficient single-pass sum frequency generation by cascaded nonlinear crystals

The cascading of nonlinear crystals has been established as a simple method to greatly increase the conversion efficiency of single-pass second-harmonic generation compared to a single-crystal scheme. Here, we show for the first time that the technique can be extended to sum frequency generation, despite differences in the phase relations of the involved fields. An unprecedented 5.5 W of continuous-wave diffraction-limited green light is generated from the single-pass sum frequency mixing of two diode lasers in two periodically poled nonlinear crystals (conversion efficiency 50%). The technique is generally applicable and can be applied to any combination of fundamental wavelengths and nonlinear crystals.
High-rate measurement-device-independent quantum cryptography
Quantum cryptography achieves a formidable task - the remote distribution of secret keys by exploiting the fundamental laws of physics. Quantum cryptography is now headed towards solving the practical problem of constructing scalable and secure quantum networks. A significant step in this direction has been the introduction of measurement-device independence, where the secret key between two parties is established by the measurement of an untrusted relay. Unfortunately, although qubit-implemented protocols can reach long distances, their key rates are typically very low, unsuitable for the demands of a metropolitan network. Here we show, theoretically and experimentally, that a solution can come from the use of continuous-variable systems. We design a coherent-state network protocol able to achieve remarkably high key rates at metropolitan distances, in fact three orders of magnitude higher than those currently achieved. Our protocol could be employed to build high-rate quantum networks where devices securely connect to nearby access points or proxy servers.

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Hybrid discrete- and continuous-variable quantum information

Research in quantum information processing has followed two different directions: the use of discrete variables (qubits) and that of high-dimensional, continuous-variable Gaussian states (coherent and squeezed states). Recently, these two approaches have been converging in potentially more powerful hybrid protocols.
Impacts of the local environment on recruitment: a comparative study of North Sea and Baltic Sea fish stocks

While the impact of environmental forcing on recruitment variability in marine populations remains largely elusive, studies spanning large spatial areas and many stocks are able to identify patterns common to different regions and species. In this study, we investigate the effects of the environment on the residuals of a Ricker stock-recruitment (SR) model, used as a proxy of prerecruits’ survival, of 18 assessed stocks in the Baltic and North Seas. A probabilistic principal components (PCs) analysis permits the identification of groups of stocks with shared variability in the prerecruits’ survival, most notably a group of pelagics in the Baltic Sea and a group composed of gadoids and herring in the North Sea. The first two PCs generally grouped the stocks according to their localizations: the North Sea, the Kattegat-Western Baltic, and the Baltic Sea. This suggests the importance of the local environmental variability on the recruitment strength. Hence, the prerecruits’ survival variability is studied according to geographically disaggregated and potentially impacting abiotic or biotic variables. Time series (1990-2009) of nine environmental variables consistent with the spawning locations and season for each stock were extracted from a physical-biogeochemical model to evaluate their ability to explain the survival of prerecruits. Environmental variables explained >70% of the survival variability for eight stocks. The variables water current, salinity, temperature, and biomass of other fish stocks are regularly significant in the models. This study shows the importance of the local environment on the dynamics of SR. The results provide evidence of the necessity of including environmental variables in stock assessment for a realistic and efficient management of fisheries.
Implementation of continuous-variable quantum key distribution with composable and one-sided-device-independent security against coherent attacks

Secret communication over public channels is one of the central pillars of a modern information society. Using quantum key distribution this is achieved without relying on the hardness of mathematical problems, which might be compromised by improved algorithms or by future quantum computers. State-of-the-art quantum key distribution requires composable security against coherent attacks for a finite number of distributed quantum states as well as robustness against implementation side channels. Here we present an implementation of continuous-variable quantum key distribution satisfying these requirements. Our implementation is based on the distribution of continuous-variable Einstein-Podolsky-Rosen entangled light. It is one-sided device independent, which means the security of the generated key is independent of any memory-free attacks on the remote detector. Since continuous-variable encoding is compatible with conventional optical communication technology, our work is a step towards practical implementations of quantum key distribution with state-of-the-art security based solely on telecom components.

General information
State: Published
Organisations: Department of Physics, Quantum Physics and Information Technology, Max-Planck-Institute für Gravitationsphysik, Leibniz Universität Hannover, University of Tokyo, Austrian Institute of Technology
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Scopus rating (2016): CiteScore 11.8 SJR 6.414 SNIP 2.855
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 6.287 SNIP 2.86 CiteScore 11.23
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 6.41 SNIP 3.034 CiteScore 10.77
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 6.206 SNIP 2.797 CiteScore 9.85
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Scopus rating (2012): SJR 5.866 SNIP 2.829 CiteScore 8.32
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
Scopus rating (2011): SJR 3.137 SNIP 1.825 CiteScore 4.44
Importance of the Reorganization Energy Barrier In Computational Design of Porphyrin-Based Solar Cells with Cobalt-Based Redox Mediators

The shift from iodide-based redox mediators in dye-sensitized solar cells toward octahedral cobalt complexes has led to a significant increase in the efficiency. However, due to the nature of this type of complexes the driving force required for the regeneration of the dye is very high, and this limits the achievable efficiency. Here we show that the large driving force is a direct consequence of the large reorganization energy of the dye regeneration reaction. The reorganization energies for charge transfer between a simple zinc porphyrin dye and two popular cobalt-based redox mediators is calculated using ab initio molecular dynamics with explicit solvent. These results are then combined with a Marcus-based extrapolation scheme to obtain the reorganization energies of more than 5000 porphyrin-based dyes. We propose a scheme for scoring the performance of the porphyrin dyes, which is able to identify already known high-performance dyes in addition to a number of even better candidates. Our analysis shows that the large internal reorganization energy of the Co-based redox mediators is an obstacle for achieving higher efficiencies.

General information
State: Published
Organisations: Center for Atomic-scale Materials Design, Department of Physics
Authors: Ørnsø, K. B. (Intern), Jónsson, E. Ö. (Intern), Jacobsen, K. W. (Intern), Thygesen, K. S. (Intern)
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Web of Science (2013): Indexed yes
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Scopus rating (2012): SJR 2.529 SNIP 1.461 CiteScore 4.98
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Improved description of metal oxide stability: Beyond the random phase approximation with renormalized kernels

The renormalized adiabatic PBE (rAPBE) method has recently been shown to comprise a significant improvement over the random phase approximation (RPA) for total energy calculations of simple solids and molecules. Here we consider the formation energies of 19 group I and II metal oxides and a few transition-metal oxides. The mean absolute error relative to experiments is 0.21 eV and 0.38 eV per oxygen atom for rAPBE and RPA, respectively, and thus the rAPBE method greatly improves the description of metal-oxygen bonds across a wide range of oxides. The failure of the RPA can be partly attributed to the lack of error cancellation between the correlation energy of the oxide on the one hand and the bulk metal and oxygen molecule on the other hand, which are all separately predicted much too negative by the RPA. We ascribe the improved performance of the rAPBE to its significantly better description of absolute correlation energies which reduces the need for error cancellation. The rAPBE is just one out of an entire class of renormalized exchange-correlation kernels which should be further investigated.
Improving performance of catalysts for water electrolysis: The MnOx case

This Ph.D. thesis presents work on non-noble metal oxide catalysts for the oxygen evolution reaction, OER. This reaction is currently a bottleneck in electrolyzer technologies, which are promising for energy storage purposes. In particular, Polymer Electrolyte Membrane, PEM, cells are attractive for decentralised hydrogen stations. PEM electrolysers rely on scarce noble metals to achieve high efficiency and durability, which limits the scalability of the technology. Finding new catalysts for OER is therefore a thriving research field with new materials being reported frequently. However, many of these new reports include little information about stability, which is evaluated solely from short term electrochemical testing. The first part of this project was therefore dedicated to designing a meaningful stability protocol. Manganese oxide thin films were prepared with sputter deposition and the stability was evaluated with Electrochemical Quartz Crystal Microbalance measurements combined with Inductively Coupled Plasma - Mass Spectrometry. The results showed that a stable electrochemical performance can be achieved, while a constant mass loss is occurring. The proposed protocol can guide future research efforts in evaluating novel materials for the OER.

Unfortunately, most non-noble metal based OER catalysts reported to this date work in alkaline solutions, where cheap NiFe electrodes are already utilized in commercial systems. For acidic media, relevant for the acidic membrane in PEM electrolysers, there is a lack of strategies aimed at designing catalysts without noble metals. It turns out that MnO2 is a stable material in the OER relevant potential range in acid. In this project, MnO2 thin films were therefore prepared to evaluate their usefulness for PEM electrolysers. Anodic dissolution of MnO2 was found to be an issue and a strategy is presented for stabilizing the surface. From density functional theory calculations it was found that titanium could segregate to surface sites prone to dissolution. Thus, MnO2 thin films were modified with titanium using a reactive co-sputtering method and tested in acid. The results indicate that the stability could be improved with more than 40 %, while the activity decreased with 10 %.

Finally, for MnO2 to be useful as an OER catalyst in PEM cells, the activity should be improved. Mixtures of manganese oxide and gold have been reported to exhibit activity enhancements and, hence, a nal part of the thesis focus on this system. Mixed thin films were prepared, which exhibited ve times higher current density compared to pure Mn oxides. X-ray Diffraction measurements indicated that Au domains of approximately 3 nm were important for this enhancement. Furthermore, from an in-situ X-ray Absorption Spectroscopy study it was found that Mn oxidises at a more cathodic potential when Au is nearby. This experimental study serves as a starting point for understanding the beneficial interaction between gold and manganese oxides.

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Authors: Frydendal, R. (Intern), Chorkendorff, I. (Intern), Stephens, I. (Intern)
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Improving the oxygen reduction reaction by strain effects: bulk and nanoparticles studies

General information
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Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics, Center for Electron Nanoscopy, Stanford University
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Publisher: Technical University of Denmark (DTU)
Influence of Adsorbed Water on the Oxygen Evolution Reaction on Oxides

We study the interface between adsorbed water and stoichiometric, defect-free (110) rutile oxide surfaces of TiO$_2$, RuO$_2$, and IrO$_2$ in order to understand how water influences the stabilities of the intermediates of the oxygen evolution reaction (OER). In our model the water is treated as explicitly adsorbed H$_2$O molecules, which are found to form two-dimensional water chains (layers) on all investigated oxide surfaces. The first chain formed by the most strongly bound H$_2$O molecules is adsorbed on the 5-fold coordinated surface metal atoms. The second chain is composed of less strongly bound H$_2$O molecules binding to bridging oxygens. The third chain interacts weakly and predominantly with the H$_2$O molecules of the second layer, resembling bulk water. We find that the stability of the water layer close to the oxide surface is almost the same as the one found on flat metal surfaces, such as the Pt(111) surface, despite the highly different adsorption pattern of the water molecules. We show that the presence of a water network has some effect on the interaction of individual intermediates of the OER with the oxide surface. However, the theoretical OER overpotential remains almost unchanged in the case of RuO$_2$ and IrO$_2$, while it is increased by similar to 0.4 eV for TiO$_2$.
Influence of ion cyclotron heating and MHD instabilities on the fast-ion distribution in ASDEX Upgrade

General information
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Organisations: Department of Physics, Plasma Physics and Fusion Energy, Max-Planck-Institut fur Plasmaphysik
Authors: Weiland, M. (Ekstern), Geiger, B. (Ekstern), Bilato, R. (Ekstern), Jacobsen, A. S. (Intern), Salewski, M. (Intern), Schneider, P. (Ekstern), Tardini, G. (Ekstern)
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Injection molded polymeric hard X-ray lenses
A novel and economical approach for fabricating compound refractive lenses for the purpose of focusing hard X-rays is described. A silicon master was manufactured by UV-lithography and deep reactive ion etching (DRIE). Sacrificial structures were utilized, which enabled accurate control of the etching profile and were removed after DRIE. By electroplating, an inverse nickel sample was obtained, which was used as a mold insert in a commercial polymer injection molding machine. A prototype lens made of polyethylene with a focal length of 350 mm was tested using synchrotron radiation at photon energies of 17 keV. A 55 µm long line focus with a minimal waist of 770 nm (FWHM) and a total lens transmittance of 32% were measured. Due to its suitability for cheap mass production, this highly efficient optics may find widespread use in hard X-ray instruments.

General information
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In situ ptychography during the annealing treatment of heterogeneous nanoporous gold catalysts

General information
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Organisations: Center for Electron Nanoscopy, Department of Physics, Experimental Surface and Nanomaterials Physics, Karlsruher Institut für Technologie, Deutsches Elektronen-Synchrotron, Technische Universität Dresden
Authors: Baier, S. (Ekstern), Benzi, F. (Ekstern), Rochet, A. (Ekstern), Scholz, M. (Ekstern), Hoppe, R. (Ekstern), Shi, J. (Ekstern), Wittstock, A. (Ekstern), Bäumer, M. (Ekstern), Damsgaard, C. D. (Intern), Schroer, C. (Ekstern), Grunwaldt, J. (Ekstern)
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In-situ STM study of sulfide adsorption on Au(100) in alkaline solution

The adsorption of sulfide on a Au(100) electrode from a 0.01 M NaOH + 0.5 mM Na2S electrolyte was studied by in situ scanning tunneling microscopy (STM) and cyclic voltammetry (CV). Starting with a sulfur free electrode surface at low potentials the subsequent formation of a p(2 × 2)-S, a c(2 × 6)-S and a c(2 × 2)-S phase was observed during potential increase. Only the p(2 × 2)-S (ΘS = 0.25 ML) phase appears as a single species phase; the c(2 × 6)-S (ΘS = 0.33 ML) and the c(2 × 2)-S (ΘS = 0. 5 ML) phase are accompanied by the simultaneous appearance of additional "dimer" particles. Concomitant changes of the step morphology and the results of the electrochemical characterization strongly suggest that these additional particles contain both, sulfur and gold atoms. Upon further potential increase the formation of a phase consisting of ring-like units was found, which is well known for Au(111) surfaces in the presence of sulfur. This phase is, by analogy, interpreted as a gold sulfide compound formed under electrochemical conditions. © 2014 Elsevier B.V. All rights reserved.
In Situ Studies of Fe$^{4+}$ Stability in $\beta$-Li$_3$Fe$_2$(PO$_4$)$_3$ 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 $\beta$-Li$_3$Fe$_2$(PO$_4$)$_3$. The work includes in situ synchrotron X-ray powder diffraction studies (XRPD) during charging of $\beta$-Li$_3$Fe$_2$(PO$_4$)$_3$ 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 $\beta$-Li$_3$Fe$_2$(PO$_4$)$_3$.

General information

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Organisations: Department of Energy Conversion and Storage, Atomic scale modelling and materials, Department of Physics, Neutrons and X-rays for Materials Physics, Applied Electrochemistry, Fundamental Electrochemistry
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Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
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BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.331 SNIP 1.335 CiteScore 2.74
ISI indexed (2011): ISI indexed yes
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BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.418 SNIP 1.304
Web of Science (2010): Indexed yes
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Scopus rating (2008): SJR 1.595 SNIP 1.41
Web of Science (2008): Indexed yes
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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
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Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 1.6 SNIP 1.846

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In situ SU-8 silver nanocomposites

Nanocomposite materials containing metal nanoparticles are of considerable interest in photonics and optoelectronics applications. However, device fabrication of such materials always encounters the challenge of incorporation of preformed nanoparticles into photoresist materials. As a solution to this problem, an easy new method of fabricating silver nanocomposites by an in situ reduction of precursors within the epoxy-based photoresist SU-8 has been developed. AgNO3 dissolved in acetonitrile and mixed with the epoxy-based photoresist SU-8 forms silver nanoparticles primarily during the pre- and post-exposure soft bake steps at 95 degrees C. A further high-temperature treatment at 300 degrees C resulted in the formation of densely homogeneously distributed silver nanoparticles in the photoresist matrix. No particle growth or agglomeration of nanoparticles is observed at this point. The reported new in situ silver nanocomposite materials can be spin coated as homogeneous thin films and structured by using UV lithography. A resolution of 5 µm is achieved in the lithographic process. The UV exposure time is found to be independent of the nanoparticle concentration. The fabricated silver nanocomposites exhibit high plasmonic responses suitable for the development of new optoelectronic and optical sensing devices.
In Situ TEM Creation of Nanowire Devices

Integration of silicon nanowires (SiNWs) as active components in devices requires that desired mechanical, thermal and electrical interfaces can be established between the nanoscale geometry of the SiNW and the microscale architecture of the device. In situ transmission electron microscopy (TEM), which has proved to be a powerful method for visualizing the physical processes involved in the growth of nanowires by the vapour liquid solid (VLS) mechanism, was used to study VLS SiNW contact formation process. Electrical characteristics and effects of surface modification on electrical behavior of SiNW were also investigated in situ.

SiNWs were grown on silicon microcantilever heaters using the VLS mechanism. When grown across a gap between adjacent cantilevers, contact was formed when the SiNW impinged on the sidewall of an adjacent cantilever. Using in situ TEM, SiNW contact formation process at high temperatures was observed in real time. As the eutectic droplet made contact, it wetted the surface; Si growth catalyzed by the eutectic continued, while at the same time Au often migrated/diffused away from the contact site. The parameters of this contact formation process were measured from movies recorded during contact events. It is demonstrated that the geometry of the final contact formed between the nanowire and the silicon surface could be controlled by varying the contact surface temperature and the electrical current through the bridging SiNW. By adjusting the contact surface temperature and nanowire current, the balance of Si deposition vs. Au migration could be controlled. This gave rise to a variety of contact geometries including a Si to Si contact with controlled shape and diameter, a nano gap, or a Si-Au-Si contact. It is further demonstrated that electromigration is the best candidate for controlling catalyst migration. Kinetics of the contact formation process was studied in detail and the conditions which resulted in different contact geometries are explained.

On completion of the contact, SiNW bridging the adjacent cantilevers was electrically connected at its two ends, base and tip and its electrical properties were probed in situ TEM. Such SiNW bridges clamped between two cantilevers in situ TEM was an interesting platform for studying the effect of surface modification on SiNWs electrical properties. The effect of surface oxidation was studied and it is demonstrated that oxidation causes substantial increase in the resistance of the nanowire.

General information
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Organisations: Department of Micro- and Nanotechnology, Molecular Windows, Department of Physics, Experimental Surface and Nanomaterials Physics, Silicon Microtechnology
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In situ XAS monitoring the formation of Pd$_2$Ga/SiO$_2$ nanoparticles for CO$_2$ hydrogenation to methanol

Methanol is a bulk chemical used as basis for many important downstream products such as formaldehyde, acetic acid and plastics. Furthermore it can be directly used as fuel. We have prepared Pd$_2$Ga/SiO$_2$ catalyst by impregnation of nitrates followed by calcination and reduction under H$_2$ atmosphere. The catalytic tests showed that at ambient pressure, the intrinsic activity of the Pd$_2$Ga/SiO$_2$ is higher than that of the conventional Cu/ZnO/Al$_2$O$_3$, while the production of the undesired CO is lower. XAS was employed to investigate the formation and local structure of Pd$_2$Ga, the results showed that the nitrates are converted to highly dispersed and disordered oxide phases which are alloyed under heating in H$_2$/Ar atmosphere giving rise to Pd$_2$Ga nanoparticles.

Integrated Quantum Optics: Experiments towards integrated quantum-light sources and quantum-enhanced sensing

The work presented in this thesis is focused on experimental application and generation of continuous variable quantum correlated states of light in integrated dielectric structures. Squeezed states are among the most exploited continuous variable optical states for free-space quantum-enhanced sensing and communication protocols, but for these developments to be applicable for future technologies they must be transformed to an integrated architecture compatible with current electro-optical technology. So far only little work has been done in this direction, but two such contributions are made in this thesis: Firstly, we present proof-of-principle demonstration of interfacing squeezed light with an on-chip optomechanical resonator, demonstrating a quantum-enhanced sensitivity to the vibrations of the micromechanical object. Secondly, work on developing an integrated source of squeezed light is presented and an optimized device design is proposed. The devices have been fabricated and tested optically and preliminary interrogations of the output quantum noise have been performed.
Integrated source of broadband quadrature squeezed light

An integrated silicon nitride resonator is proposed as an ultracompact source of bright single-mode quadrature squeezed light at 850 nm. Optical properties of the device are investigated and tailored through numerical simulations, with particular attention paid to loss associated with interfacing the device. An asymmetric double layer stack waveguide geometry with inverse vertical tapers is proposed for efficient and robust fibre-chip coupling, yielding a simulated total loss of -0.75 dB/facet. We assess the feasibility of the device through a full quantum noise analysis and derive the output squeezing spectrum for intra-cavity pump self-phase modulation. Subject to standard material loss and detection efficiencies, we find that the device holds promises for generating substantial quantum noise squeezing over a bandwidth exceeding 1 GHz. In the low-propagation loss regime, approximately -6 dB squeezing is predicted for a pump power of only 75 mW.

General information
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Organisations: Department of Physics, Quantum Physics and Information Technology
Authors: Hoff, U. B. (Intern), Nielsen, B. M. (Intern), Andersen, U. L. (Intern)
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Journal: Optics Express
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Scopus rating (2017): SJR 1.519 SNIP 1.567 CiteScore 3.74
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.48 SJR 1.532 SNIP 1.544
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.91 SNIP 1.674 CiteScore 3.78
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.313 SNIP 2.124 CiteScore 4.18
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.337 SNIP 2.196 CiteScore 4.38
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 2.562 SNIP 2.108 CiteScore 3.85
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 2.58 SNIP 2.572 CiteScore 4.04
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 2.906 SNIP 2.428
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 3.039 SNIP 2.679
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 3.204 SNIP 2.423
Interactions of a zwitterionic thiophene-based conjugated polymer with surfactants

In this paper we investigate the optical and structural properties of a zwitterionic poly[3-(N-(4-sulfonato-1-butyl)-N,N-diethylammonium)hexyl-2,5-thiophene] (P3SBDEAHT) conjugated polyelectrolyte (CPE) and its interaction in water with surfactants, using absorption, photoluminescence (PL), electrical conductivity, molecular dynamics simulations (MDS) and small-angle X-ray scattering (SAXS). Different surfactants were studied to evaluate the effect of the head group and chain length on the self-assembly. PL data emphasize the importance of polymer-surfactant electrostatic interactions in the formation of complexes. Nevertheless, conductivity and MDS data have shown that nonspecific interactions also play an important role. These seem to be responsible for the spatial position of the surfactant tail in the complex and, eventually, for breaking-up P3SBDEAHT aggregates. SAXS measurements on P3SBDEAHT-zwitterionic cocamidopropyl betaine (CAPB) surfactant complexes showed a specific structural organization of the system. The CAPB surfactant promotes a structural transition from pure P3SBDEAHT 3-dimensional aggregates (radius of gyration ~85 Å) to thick cylindrical aggregates (~20 Å) where all CAPB molecules are associated with the polymer. For molar ratios (in terms of the polymer repeat unit) >1 the SAXS interference maximum of the complexes resembles that of pure CAPB thus suggesting ongoing phase segregation in the formation of a "pure" CAPB phase.

General information

State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Bergische Universität Wuppertal, University of Coimbra
Number of pages: 11
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Publication date: 2015
Main Research Area: Technical/natural sciences

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Journal: Polymer Chemistry
Volume: 6
Issue number: 46
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BFI (2018): BFI-level 1
Intercellular communication via plasmodesmata

General information
State: Published
Organisations: Department of Physics, Biophysics and Fluids, The Institute of Chemical and Physical Research, University of Edinburgh
Authors: Kitagawa, M. (Ekstern), Paultre, D. (Ekstern), Rademaker, H. (Intern)
Number of pages: 3
Pages: 970-972
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
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Volume: 205
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ISSN (Print): 0028-646X
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): SNIP 2.153 SJR 3.787 CiteScore 6.65
Web of Science (2017): Indexed yes
Interfacing transitions of different alkali atoms and telecom bands using one narrowband photon pair source

Quantum information technology strongly relies on the coupling of optical photons with narrowband quantum systems, such as quantum dots, color centers, and atomic systems. This coupling requires matching the optical wavelength and bandwidth to the desired system, which presents a considerable problem for most available sources of quantum light.
Here we demonstrate the coupling of alkali dipole transitions with a tunable source of photon pairs. Our source is based on spontaneous parametric downconversion in a triply resonant whispering gallery mode resonator. For this, we have developed novel wavelength-tuning mechanisms that allow a coarse tuning to either the cesium or rubidium wavelength, with subsequent continuous fine-tuning to the desired transition. As a demonstration of the functionality of the source, we performed a heralded single-photon measurement of the atomic decay. We present a major advance in controlling the spontaneous downconversion process, which makes our bright source of heralded single photons now compatible with a plethora of narrowband resonant systems.

Intermetallic GaPd₂ Nanoparticles on SiO₂ for Low-Pressure CO₂ Hydrogenation to Methanol: Catalytic Performance and In Situ Characterization

A nanodispersed intermetallic GaPd₂/SiO₂ catalyst is prepared by simple impregnation of industrially relevant high-surface-area SiO₂ with Pd and Ga nitrate, followed by drying, calcination, and reduction in hydrogen. The catalyst is tested for CO₂ hydrogenation to methanol at ambient pressure, revealing that the intrinsic activity of the GaPd₂/SiO₂ is higher than that of the conventional Cu/ZnO/Al₂O₃, while the production of the undesired CO is lower. A combination of complementary in situ and ex situ techniques are used to investigate the GaPd₂/SiO₂ catalyst. In situ X-ray diffraction and in situ extended X-ray absorption fine structure spectroscopy show that the GaPd₂ intermetallic phase is formed upon activation of the catalyst via reduction and remains stable during CO₂ hydrogenation. Identical location-transmission electron microscopy images acquired ex situ (i.e., micrographs of exactly the same catalyst area recorded at the different steps of activation and reaction procedure) show that nanoparticle size and dispersion are defined upon calcination with no significant changes observed after reduction and methanol synthesis. Similar conclusions can be drawn from electron diffraction patterns and images acquired using environmental TEM (ETEM), indicating that ETEM results are representative for the catalyst treated at ambient pressure. The chemical composition and the crystalline structure of the nanoparticles are identified by scanning TEM energy dispersive X-ray spectroscopy, selected area electron diffraction, and atomically resolved TEM images.
(Invited) Microreactors for Characterization and Benchmarking of Photocatalysts


General Information
State: Published
Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics, Department of Structural Engineering and Materials, Japan Technological Research Association of Artificial Photosynthetic Chemical Process, Tokyo Institute of Technology
Number of pages: 1
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Main Research Area: Technical/natural sciences

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Journal: Electrochemical Society. Meeting Abstracts (Online)
Volume: MA2015-01
Issue number: 27
Article number: 1611
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http://ma.ecsd.org/content/MA2015-01/27/1611.abstract?sid=dacbea93-e422-4d57-84be-101c69853a9a
Source: FindIt
Source-ID: 274863120
Publication: Research - peer-review › Conference abstract in journal – Annual report year: 2015

(Invited) Towards the Development of Active, Stable and Abundant Catalysts for Oxygen Evolution in Acid

Of the different water splitting technologies, polymer electrolyte membrane (PEM) electrolysers are the most amenable towards small-scale delocalized storage of renewable electricity. In order for these devices make a significant impact to the global energy landscape, they will need to be scaled to the TW level. State-of-the-art PEM electrolysers employ IrOx, which is both expensive and scarce, to catalyse oxygen evolution.(1) Around a decade’s worth of Ir production would be required to scale up PEM electrolysis to the TW scale: this is clearly untenable.(2) It turns out that RuOx has a higher catalytic activity than IrOx, but is more prone to dissolution.(3-5) All other surfaces are completely inactive or unstable. We recently demonstrated that mass-selected RuOx nanoparticles exhibited an order of magnitude improvements in both mass activity and turnover frequency over the state of the art. Should this activity be stabilised for instance, by utilising a more stable oxide such as TiOx or IrOx,(6, 7) PEM electrolysis could indeed be scalable to the TW level. Alternatively, the precious metal catalysts could be eliminated altogether and replaced by abundant, active and stable catalysts. However, this is not a trivial task, given the highly oxidising and corrosive environment under reaction conditions. Herein, we attempt to address this problem by stabilising MnOx with TiOx. Density functional theory calculations suggest that the undercoordinated surface sites on MnOx, which are inactive and also most prone to dissolution, could be stabilised by TiOx. We test this notion by performing oxygen evolution on Mn-TiOx thin films. We probe the composition using X-ray photoelectron spectroscopy measurements and dissolution with inductively coupled plasma mass spectroscopy. We confirm that TiOx does indeed engender MnOx with modest stability. Further development of this strategy opens up the possibility of developing active, stable and abundant non-precious metal oxides for oxygen evolution in acid. References 1. M. K. Debe, S. M. Hendricks, G. D. Vernstrom, M. Meyers, M. Brostrom, M. Stephens, Q. Chari, J. Willey, M. Hamden, C. K. Mittelstedt, C. B. Capuano, K. E. Ayers and E. B. Anderson, J. Electrochem. Soc., 159, K165 (2012). 2. E. A. Paoli, F. Masini, R. Frydendal, D. Deiana, C. Schlaup, M. Malizia, T. W. Hansen, S. Horch, I. E. L. Stephens and I. Chorkendorff, Chemical Science, DOI: 10.1039/c4sc02685c (2015). 3. T. Reier, M. Oezaslan and P. Strasser, ACS Catalysis, 2, 1765
Iron sensitizer converts light to electrons with 92% yield

Solar energy conversion in photovoltaics or photocatalysis involves light harvesting, or sensitization, of a semiconductor or catalyst as a first step. Rare elements are frequently used for this purpose, but they are obviously not ideal for large-scale implementation. Great efforts have been made to replace the widely used ruthenium with more abundant analogues like iron, but without much success due to the very short-lived excited states of the resulting iron complexes. Here, we describe the development of an iron-nitrogen-heterocyclic-carbene sensitizer with an excited-state lifetime that is nearly a thousand-fold longer than that of traditional iron polypyridyl complexes. By the use of electron paramagnetic resonance, transient absorption spectroscopy, transient terahertz spectroscopy and quantum chemical calculations, we show that the iron complex generates photoelectrons in the conduction band of titanium dioxide with a quantum yield of 92% from the 3 MLCT (metal-to-ligand charge transfer) state. These results open up possibilities to develop solar energy-converting materials based on abundant elements.
Ketene as a Reaction Intermediate in the Carbonylation of Dimethyl Ether to Methyl Acetate over Mordenite

Unprecedented insight into the carbonylation of dimethyl ether over Mordenite is provided through the identification of ketene (CH$_2$CO) as a reaction intermediate. The formation of ketene is predicted by detailed DFT calculations and verified experimentally by the observation of doubly deuterated acetic acid (CH$_2$DCOOD), when D$_2$O is introduced in the feed during the carbonylation reaction.

**General information**

State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, Center for Atomic-scale Materials Design, Department of Physics, Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Haldor Topsoe AS, SUNCAT Center for Interface Science and Catalysis
Authors: Rasmussen, D. B. (Intern), Christensen, J. M. (Intern), Temel, B. (Intern), Studt, F. (Intern), Moses, P. G. (Intern), Rossmeisl, J. (Intern), Riisager, A. (Intern), Jensen, A. D. (Intern)
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Web of Science (2018): Indexed yes
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Web of Science (2017): Indexed yes
Carbonylation, Density functional calculations, Heterogeneous catalysis, Reaction mechanisms, Zeolites

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Source: FindIt
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Publication: Research - peer-review › Journal article – Annual report year: 2015
Ketene as a Reaction Intermediate in the Carbonylation of Dimethyl Ether to Methyl Acetate over Mordenite

Unprecedented insight into the carbonylation of dimethyl ether over Mordenite is provided through the identification of ketene (CH2CO) as a reaction intermediate. The formation of ketene is predicted by detailed DFT calculations and verified experimentally by the observation of doubly deuterated acetic acid (CH2DCOOD), when D2O is introduced in the feed during the carbonylation reaction.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, Center for Atomic-scale Materials Design, Department of Physics, Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Haldor Topsoe AS, SUNCAT Center for Interface Science and Catalysis
Authors: Rasmussen, D. B. (Intern), Christensen, J. M. (Intern), Temel, B. (Intern), Studt, F. (Intern), Moses, P. G. (Intern), Rossmeisl, J. (Intern), Riisager, A. (Intern), Jensen, A. D. (Intern)
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Main Research Area: Technical/natural sciences

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Journal: Angewandte Chemie
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BFI (2016): BFI-level 1
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
BFI (2014): BFI-level 1
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
ISI indexed (2013): ISI indexed no
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
ISI indexed (2012): ISI indexed no
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
ISI indexed (2011): ISI indexed no
BFI (2010): BFI-level 1
BFI (2009): BFI-level 1
BFI (2008): BFI-level 1
Web of Science (2006): Indexed yes
Original language: English
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Light for Life: International Year of Light 2015

General information
State: Published
Organisations: Department of Physics, Department of Photonics Engineering, Diode Lasers and LED Systems, Leibniz Institute of Photonic Technology Jena, Medical University of Vienna, Duke University, Lund University Hospital
Authors: Leitgeb, R. A. (Ekstern), Andersen, P. E. (Intern), Popp, J. (Ekstern), Ramanujam, N. (Ekstern), Svanberg, K. (Ekstern)
Number of pages: 3
Publication date: 2015
Longitudinal domain wall formation in elongated assemblies of ferromagnetic nanoparticles

Through evaporation of dense colloids of ferromagnetic ~13 nm ε-Co particles onto carbon substrates, anisotropic magnetic dipolar interactions can support formation of elongated particle structures with aggregate thicknesses of 100-400 nm and lengths of up to some hundred microns. Lorenz microscopy and electron holography reveal collective magnetic ordering in these structures. However, in contrast to continuous ferromagnetic thin films of comparable dimensions, domain walls appear preferentially as longitudinal, i.e., oriented parallel to the long axis of the nanoparticle assemblies. We explain this unusual domain structure as the result of dipolar interactions and shape anisotropy, in the absence of inter-particle exchange coupling.

General information
State: Published
Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics, Center for Electron Nanoscopy, Center for Atomic-scale Materials Design, Institut Català de Nanotecnologia
Authors: Varón, M. (Intern), Beleggia, M. (Intern), Jordanovic, J. (Intern), Schiøtz, J. (Intern), Kasama, T. (Intern), Puntes, V. F. (Ekstern), Frandsen, C. (Intern)
Number of pages: 7
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Main Research Area: Technical/natural sciences

Publication information
Journal: Scientific Reports
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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
Massive stars formed in atomic hydrogen reservoirs: H i observations of gamma-ray burst host galaxies

Long gamma-ray bursts (GRBs), among the most energetic events in the Universe, are explosions of massive and short-lived stars, so they pinpoint locations of recent star formation. However, several GRB host galaxies have recently been found to be deficient in molecular gas (H_2), believed to be the fuel of star formation. Moreover, optical spectroscopy of GRB afterglows implies that the molecular phase constitutes only a small fraction of the gas along the GRB line of sight. Here we report the first ever 21 cm line observations of GRB host galaxies, using the Australia Telescope Compact Array, implying high levels of atomic hydrogen (H I), which suggests that the connection between atomic gas and star formation is stronger than previously thought. In this case, it is possible that star formation is directly fuelled by atomic gas (or that the H I-to-H_2 conversion is very efficient, which rapidly exhaust molecular gas), as has been theoretically shown to be possible. This can happen in low-metallicity gas near the onset of star formation because cooling of gas (necessary for star formation) is faster than the H I-to-H_2 conversion. Indeed, large atomic gas reservoirs, together with low molecular gas masses, stellar, and dust masses are consistent with GRB hosts being preferentially galaxies which have very recently started a star formation episode after accreting metal-poor gas from the intergalactic medium. This provides a natural route for forming GRBs in low-metallicity environments. The gas inflow scenario is also consistent with the existence of the companion HI object with no optical counterpart ∼19 kpc from the GRB 060505 host, and with the fact that the HI centroids of the GRB 980425 and 060505 hosts do not coincide with optical centres of these galaxies, but are located close to the GRB positions.
Materials characterisation tools towards lead-free piezoceramics

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, University of New South Wales
Authors: Oddershede, J. (Intern), Majkut, M. (Intern), Yap, E. (Ekstern), Daniels, J. (Ekstern), Schmidt, S. (Intern)
Number of pages: 1
Publication date: 2015

Host publication information
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Place of publication: Lyngby
Publisher: Technical University of Denmark (DTU)
Article number: M-3
Main Research Area: Technical/natural sciences
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Electronic versions:
M3_DTU_Sustain_2015.pdf
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2015

Mathematical beauty in service of deep approach to learning
In the fall of 2014 I taught '02601 Introduction to Numerical Algorithms' to a class of 86 engineering students at Technical University of Denmark. The course employed basic calculus and linear algebra to elucidate and analyse canonical algorithms of scientific computing. A major part of the course was hands-on MATLAB programming, where the algorithms were tested and applied to solve physical model-based problems. To encourage a deep approach, and discourage a surface approach to learning, I introduced into the lectures a basic but rigorous mathematical treatment of crucial theoretical points, emphasising the beauty of the underlying mathematical structure. Into this I integrated frequent and activating dialogue with the students. In section 1 I describe the course and the students in more detail. Section 2 details and justifies the pedagogical elements I introduced into the lectures; my central hypothesis is also given there. The results of the experiment are presented and discussed in section 3.

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Scientific Computing, Department of Physics, Neutrons and X-rays for Materials Physics
Authors: Karamehmedovic, M. (Intern)
Number of pages: 8
Publication date: 2015

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Title of host publication: Proceedings of the 43rd Annual SEFI Conference (2015)
Article number: 55856
BFI conference series: European Society for Engineering Education. Annual Conference proceedings (5010018)
Main Research Area: Technical/natural sciences
Conference: 43rd Annual Conference of the European Society for Engineering Education (SEFI 2015), Orléans, France, 29/06/2015 - 29/06/2015
Mathematics, Engineering
Electronic versions:
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Links:
http://www.sefi.be/?page_id=6043

Bibliographical note
CHAPTER 3. Mathematics and Engineering Education
Source: PublicationPreSubmission
Source-ID: 112235359
Publication: Research - peer-review › Article in proceedings – Annual report year: 2015

McStas and Mantid integration
McStas and Mantid are two well-established software frameworks within the neutron scattering community. McStas has been primarily used for simulating the neutron transport mechanisms in instruments, while Mantid has been primarily used for data reduction. We report here the status of our work done on the interoperability between the instrument simulation
software McStas and the data reduction software Mantid. This provides a demonstration of how to successfully link
together two software packages that otherwise have been developed independently, and in particular here show how this
has been achieved for an instrument simulation software and a data reduction software. This paper will also provide
examples of some of the expected future enhanced analysis that can be achieved from combining accurate instrument
and sample simulations with software for correcting raw data. The main application of this work is to treat raw data
collected at large scale neutron facilities.

**General information**

State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Rutherford Appleton Laboratory,
European Spallation Source ESS AB
Authors: Nielsen, T. R. (Ekstern), Markvardsen, A. J. (Ekstern), Willendrup, P. K. (Intern)
Number of pages: 14
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BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 0.425 SJR 0.283 CiteScore 0.53
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 0.85 SJR 0.286 SNIP 1.219
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.286 SNIP 1.92 CiteScore 0.88
BFI (2014): BFI-level 1
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
ISI indexed (2013): ISI indexed no
BFI (2012): BFI-level 1
ISI indexed (2012): ISI indexed no
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.327 SNIP 2.092
ISI indexed (2011): ISI indexed no
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.18 SNIP 0.274
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.177 SNIP 0.545
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.293 SNIP 0.424
Scopus rating (2007): SJR 0.216 SNIP 0.303
Scopus rating (2006): SJR 0.3 SNIP 0.607
Scopus rating (2005): SJR 0.205 SNIP 0.323
Scopus rating (2004): SJR 0.229 SNIP 0.458
Scopus rating (2003): SJR 0.19 SNIP 0.41
Scopus rating (2002): SJR 0.468 SNIP 0.845
Scopus rating (2001): SJR 0.324 SNIP 0.611
Scopus rating (2000): SJR 0.572 SNIP 1.108
Scopus rating (1999): SJR 0.344 SNIP 0.71
Original language: English
Data reduction, Instrumentation, Monte Carlo simulation, Neutron scattering, Ray-tracing

DOI: 10.3233/JNR-160026
Measurement and interpretation of active Balmer alpha spectra at ASDEX Upgrade

General information
State: Published
Organisations: Department of Physics, Plasma Physics and Fusion Energy, Max Planck Institute for Plasma Physics
Authors: Geiger, B. (Ekstern), Dux, R. (Ekstern), Dunne, M. (Ekstern), Lebschy, A. (Ekstern), McDermott, R. (Ekstern), Reimer, R. (Ekstern), Salewski, M. (Intern), Tardini, G. (Ekstern), Weiland, M. (Ekstern)
Number of pages: 4
Publication date: 2015

Host publication information
Title of host publication: Proceedings of the 42nd European Physical Society Conference on Plasma Physics
Publisher: European Physical Society
Main Research Area: Technical/natural sciences
Conference: 42nd European Physical Society Conference on Plasma Physics, Lisbon, Portugal, 22/06/2015 - 22/06/2015
Source: PublicationPreSubmission
Source-ID: 112051303
Publication: Research - peer-review › Article in proceedings – Annual report year: 2015

Measurement of strain in InGaN/GaN nanowires and nanopyramids
The growth and optoelectronic properties of core-shell nanostructures are influenced by the strain induced by the lattice mismatch between core and shell. In contrast with planar films, nanostructures contain multiple facets that act as independent substrates for shell growth, which enables different relaxation mechanisms. In this study, X-ray diffraction data are presented that show that InGa1-N shells grown on GaN cores are strained along each of the facets independently. Reciprocal space maps reveal multiple Bragg peaks, corresponding to different parts of the shell being strained along the individual facet planes. The strained lattice constants were found from the positions of the Bragg peaks. Vegard's law and Hooke's law for an anisotropic medium were applied in order to find the composition and strain in the InGaN shells. A range of nanowire samples with different InGaN shell thicknesses were measured and it is concluded that, with an In concentration of around 30%, major strain relaxation takes place when the thickness reaches 23nm. InGaN shells of 6 and 9nm thickness remain nearly fully strained biaxially along each of the facets of the nanowires and the facets of the nanopyramids.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, University of Copenhagen, Glo-USA Inc., GLO AB, Lund University
Authors: Stankevic, T. (Ekstern), Mickevicius, S. (Ekstern), Nielsen, M. S. (Ekstern), Kryliouk, O. (Ekstern), Ciechonski, R. (Ekstern), Vescovi, G. (Ekstern), Bi, Z. (Ekstern), Mikkelsen, A. (Ekstern), Samuelson, L. (Ekstern), Gundlach, C. (Intern), Feidenhans'l, R. K. (Ekstern)
Number of pages: 6
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Main Research Area: Technical/natural sciences

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Volume: 48
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Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 1.346 SJR 1.635 CiteScore 2.72
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
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BFI (2008): BFI-level 2
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Scopus rating (2006): SJR 2.164 SNIP 7.401
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Scopus rating (2001): SJR 1.808 SNIP 2.194
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Measurements of 3D slip velocities and plasma column lengths of a gliding arc discharge

A non-thermal gliding arc discharge was generated at atmospheric pressure in an air flow. The dynamics of the plasma column and tracer particles were recorded using two synchronized high-speed cameras. Whereas the data analysis for such systems has previously been performed in 2D (analyzing the single camera image), we provide here a 3D data analysis that includes 3D reconstructions of the plasma column and 3D particle tracking velocimetry based on discrete tomography methods. The 3D analysis, in particular, the determination of the 3D slip velocity between the plasma column and the gas flow, gives more realistic insight into the convection cooling process. Additionally, with the determination of the 3D slip velocity and the 3D length of the plasma column, we give more accurate estimates for the drag force, the electric field strength, the power per unit length, and the radius of the conducting zone of the plasma column. © 2015 AIP Publishing LLC.
Measurements of the fast-ion distribution function at ASDEX upgrade by collective Thomson scattering (CTS) using active and passive views

Collective Thomson scattering (CTS) can provide measurements of the confined fast-ion distribution function resolved in space, time and 1D velocity space. On ASDEX Upgrade, the measured spectra include an additional signal which previously has hampered data interpretation. A new set-up using two independent heterodyne receiver systems enables subtraction of the additional part from the total spectrum, revealing the resulting CTS spectrum. Here we present CTS measurements from the plasma centre obtained in L-mode and H-mode plasmas with and without neutral beam injection (NBI). For the first time, the measured spectra agree quantitatively with the synthetic spectra in periods with and without NBI heating. For the discharges investigated, the central velocity distribution of neutral beam ions can be described by classical slowing down. These results will have a major impact on ITER physics exploration, since CTS is presently the only diagnostic to measure the confined alpha particles produced by the fusion reactions.
Mechanistic Pathway in the Electrochemical Reduction of CO₂ on RuO₂
RuO₂ has been reported to reduce CO₂ electrochemically to methanol at low overpotential. Herein, we have used density functional theory (DFT) to gain insight into the mechanism for CO₂ reduction on RuO₂(110). We have investigated the thermodynamic stability of various surface terminations in the electrochemical environment and found CO covered surfaces to be particularly stable, although their formation might be kinetically limited under mildly reducing conditions. We have identified the lowest free energy pathways for CO₂ reduction to formic acid (HCOOH), methanol (CH₃OH), and methane (CH₄) on partially reduced RuO₂(110) covered with 0.25 and 0.5 ML of CO*. We have found that CO₂ is reduced to formic acid, which is further reduced to methanol and methane. At 0.25 ML of CO*, the reduction of formate (OCHO*) to formic acid is the thermodynamically most difficult step and becomes exergonic at potentials below −0.43 V vs the reversible hydrogen electrode (RHE). On the other hand, at 0.5 ML of CO*, the reduction of formic acid to H₂COOH* is the thermodynamically most difficult step and becomes exergonic at potentials below −0.25 V vs RHE. We have found that CO₂ reduction activity on RuO₂ changes with CO coverage, which suggests that CO coverage can be used as a tool to tune the CO₂ reduction activity. We have shown the mechanism for CO₂ reduction on RuO₂ to be different from that on Cu. On Cu, hydrocarbons are formed at high Faradaic efficiency through reduction of CO* at ∼1 V overpotential, while on RuO₂, methanol and formate are formed through reduction of formic acid at lower overpotentials. Using our understanding of the CO₂ reduction mechanism on RuO₂, we suggest reduction of formic acid on RuO₂, which should lead to methanol and methane production at relatively low overpotentials.
Membrane technologies for water treatment and reuse in the textile industry

Textile wastewater is a challenging feed stream for treatment by membrane separation because of its complex composition and the presence of reactive components. Here we briefly present examples of reverse osmosis-, nanofiltration- and ultrafiltration-based systems as well as membrane bioreactor technology for textile wastewater remediation. However, for all of these approaches the general issue of (bio)fouling represents a major obstacle for full-scale industrial implementation. Forward osmosis (FO) membranes have recently attracted considerable interest because the low fouling propensity of FO membranes makes them an intriguing supplement to existing methods. We present the FO principle with some current FO membrane developments including biomimetic aquaporin FO membranes, and exemplify how they can be used to concentrate textile dyes.

Methods to determine fast-ion distribution functions from multi-diagnostic measurements

Understanding the behaviour of fast ions in a fusion plasma is very important, since the fusion-born alpha particles are expected to be the main source of heating in a fusion power plant. Preferably, the entire fast-ion velocity-space distribution function would be measured. However, no fast-ion diagnostic is capable of measuring the entire distribution function. The velocity space sensitivity of a fast-ion diagnostic is given by so-called velocity-space weight functions. Here, the development of neutron emission spectrometry weight functions is presented. By combining measurements from several fast-ion diagnostic views, it is possible to infer the distribution function using a tomography approach. Several inversion methods for solving this tomography problem in velocity space are implemented and compared. It is found that the best quality it obtained when using inversion methods which penalise steep gradients in the velocity-space distribution function. The different inversion methods are used to study actual fast-ion measurements from the ASDEX Upgrade tokamak. By calculating tomographies of the distribution before and after a sawtooth crash, it is possible to identify the parts of velocity-space where the fast ions are affected the most. Finally, the first ever tomographies calculated using a combination of measurements from different types of fast-ion diagnostics are presented.
Microfabrication and testing of refractive hard X-ray optics

General information
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Microfabrication of hard x-ray lenses
This thesis deals with the development of silicon compound refractive lenses (Si-CRLs) for shaping hard x-ray beams. The CRLs are to be fabricated using state of the art microfabrication techniques. The primary goal of the thesis work is to produce Si-CRLs with considerably increased structure heights and improved uniformity compared to what is currently available. To this end, established fabrication procedures are improved and the toolbox used for lens development is enriched.

The central theme of this thesis is x-ray microscopy (XRM). As a spearhead of today’s materials research it provides characterization details that cannot be obtained by other means. The respective x-ray techniques largely benefit from continuously improved x-ray lenses, x-ray detectors and x-ray optics. For instance, some techniques aiming for structural investigation of poly-crystalline materials directly benefit from more intense and wider line beams with narrower waists. The thesis starts with a review of alternative x-ray lenses. Si-CRLs are identified as valuable optical components that allow shaping hard x-rays efficiently and creating beam waists that are clearly in the nanometer range. They stand out by their potential for compact integration, which makes them cost-effective, easy to handle and stable on-axis optics.

A Si-CRL comprises multiple bi-parabolic cylindrical cavities. The bi-parabolic patterns are defined lithographically and vertically transferred into the Si substrate using deep reactive ion etching (DRIE). Based on a theoretical framework for CRLs, stringent requirements on the pattern transfer are found. Most crucially, the sidewalls of the cavities must be strictly parallel. Already slight deviations from the ideal parabolic shapes result in non-uniform and broadened waists of focused x-ray beams.

Two strategies are demonstrated, which guarantee shape fidelity, while the heights of etched lenses can be increased. Both are based on defining the bi-parabolic cavities at their perimeter by trenches of uniform width, where one trench wall is comprised of sacrificial material. The two strategies differ in the way the unwanted sacrificial material inside the cavities is removed subsequent to DRIE. While the first strategy utilizes etching of the trenches through the entire thickness of the wafer for releasing the sacrificial portions, the second strategy relies on thin sacrificial structures that can be completely oxidized and removed by selective etching. Both strategies have proven to be equally successful in achieving a substantial increase of the heights of Si-CRLs and to facilitate accurate sidewall profile control necessary for uniform x-ray focusing. A precise manufacture in turn asks for highly precise metrology. Therefore, a mix of techniques including optical profilometry and atomic force microscopy (AFM) has been used to obtain reliable information about the detailed three-dimensional shapes of the lenses. Adequate sample preparation and measuring procedures have been developed. Inverse replica molding in PDMS of the CRLs was established as an effective way to circumvent the limitations AFM probes have when concave surfaces need to be characterized, e.g. due to the finite lengths of AFM probes.

Four different x-ray optical components have been designed, manufactured and characterized with respect to their shape. Their optical performances were tested at the European Synchrotron Radiation Facility (ESRF). Two 1D-focusing Si-CRLs suitable as condensers in hard-XRM were developed utilizing the aforementioned two different strategies. The first Si-condenser showed focusing of a 56 keV x-ray beam into a 310 μm wide line and a waist of 980 nm (FWHM, full width at half maximum) at a focal length of 1.3 m. The second Si-condenser allowed the focusing of 17 keV x-rays into a 180 μm-wide line with a waist of 430 nm (FWHM) at a focal length of 0.215 m. Both systems leave plenty of space for sample
surroundings and ensure low-divergent and wide x-ray beams with narrow waists. Both results are substantial improvements to what was available at the start of this thesis work.

The challenge of making x-ray objectives in silicon by interdigitation of lenslets alternately focusing in the vertical and horizontal directions was addressed. A functioning prototype of a 2D silicon objective for use in a bright-field hard-XRM was demonstrated. The results are promising; showing acceptably low aberration and performance close to theoretical expectations. A resolution of 300 nm with 17 keV x-rays and a focal length of 300 mm was achieved. By harnessing the potential for making more compact objectives and avoiding shape defects, one could significantly improve the focusing power, transmission and numerical aperture.

Polymer injection molding was explored as a novel route for x-ray lens manufacture. A Si-CRL template was used as a master for obtaining nickel mold inserts. CRLs made of polyethylene have proven to be promising highly efficient x-ray optics. A 55 μm long line focus with a minimal waist of 770 nm (FWHM) at a focal length of 350 mm was obtained with 17 keV x-rays. A final production rate larger than 10 pieces per hour indicates the economic value of injection molded x-ray lenses, which may have applications in more readily available small laboratory x-ray instruments or medical devices.

In each case, observed non-uniformities of the shaped x-ray beams were investigated and found to be in agreement with the lens shape measurements. In iterative steps the lenses have been improved and the most recent results allow yet another whole range of improvements to be made. The fundamentals for an advanced fabrication of silicon CRLs are laid out, which will contribute to their future use in novel applications.

Microstructure and micromechanics of the heart urchin test from X-ray tomography

The microstructure of many echinoid species has long fascinated scientists because of its high porosity and outstanding mechanical properties. We have used X-ray microtomography to examine the test of Echinocardium cordatum (heart urchin), a burrowing cousin of the more commonly known sea urchins. Three dimensional imaging demonstrates that the bulk of the test is composed of only two distinct, highly porous, fenestrated regions (stereom), in which the thickness of the struts is constant. Different degrees of porosity are achieved by varying the spacing of the struts. Drawing an analogy to vertebrate trabecular bone, where for example, human bone has a connectivity density of ≈1/mm³, we measure up to 150,000 strut connections per mm³. Simulations of mechanical loading using finite element calculations indicate that the test performs at very close to the optimum expected for foams, highlighting the functional link between structure and mechanical properties.
We present calculations of the phonon-limited mobility in intrinsic n-type monolayer graphene, silicene and MoS$_2$. The material properties, including the electron-phonon interaction, are calculated from first principles. Unlike graphene, the carriers in silicene show strong interaction with the out-of-plane modes. However, we find that graphene only has a slightly higher mobility compared to silicene. For MoS$_2$, we obtain several orders of magnitude lower mobilities and in agreement with other recent theoretical results. The simulations illustrate the predictive capabilities of the newly implemented Boltzmann Transport Equation (BTE) solver in the Atomistix ToolKit (ATK) simulation tool.
Modeling light–tissue interaction in optical coherence tomography systems

Optical coherence tomography (OCT) performs high-resolution, cross-sectional tomographic imaging of the internal tissue microstructure by measuring backscattered or backreflected light. The scope of this chapter is to present analytical and numerical models that are able to describe light–tissue interactions and its influence on the performance of OCT systems including multiple scattering effects in heterogeneous media. In general, these models, analytical as well as numerical, may serve as important tools for improving interpretation of OCT images and also serve as prerequisites for extraction of tissue optical scattering parameters.

Morphological instability during steady electrodeposition at overlimiting currents

We present a linear stability analysis of a planar metal electrode during steady electrodeposition. We extend the previous work of Sundstrom and Bark by accounting for the extended space-charge density, which develops at the cathode once the applied voltage exceeds a few thermal voltages. In accordance with Chazalviel's conjecture, the extended space-charge region is found to greatly affect the morphological stability of the electrode. To supplement the numerical solution of the stability problem, we have derived analytical expressions valid in the limit of low and high voltage, respectively.
Morphology of Copper Tin Sulfide Films Grown by Pulsed Laser Deposition at 248 and 355 nm

Thin films solar cells based on Cu2ZnSnS4 (CZTS) as absorber layer have seen a rapid development leading to a world record of 8.8% [1]. However, other p-type semiconductors with fewer elements and reduced complexity compared to CZTS are also available, such as ternary Cu–Sn–S systems, i.e. Cu2SnS3 (CTS) [2].

Mössbauer, SANS and magnetic characterization of interacting iron oxide nanoparticles (IONPs)

Multiphoton imaging with a novel compact diode-pumped Ti:sapphire oscillator

Multiphoton laser scanning microscopy commonly relies on bulky and expensive femtosecond lasers. We integrated a novel minimal-footprint Ti:sapphire oscillator, pumped by a frequency-doubled distributed Bragg reflector tapered diode laser, into a clinical multiphoton tomograph and evaluated its imaging capability using different biological samples, i.e. cell monolayers, corneal tissue, and human skin. With the novel laser, the realization of very compact Ti:sapphire-based systems for high-quality multiphoton imaging at a significantly size and weight compared to current systems will become possible.
Multistability and hidden attractors in a multilevel DC/DC converter

An attracting periodic, quasiperiodic or chaotic set of a smooth, autonomous system may be referred to as a “hidden attractor” if its basin of attraction does not overlap with the neighborhood of an unstable equilibrium point. Historically, this condition has implied that the basin of attraction for the hidden set in most cases has been so complicated that special analytic and/or numerical techniques have been required to locate the set. By simulating the model of a multilevel DC/DC converter that operates in the regime of high feedback gain, the paper illustrates how pulse-width modulated control can produce complicated structures of attracting and repelling states organized around the basic switching cycle. This leads us to suggest the existence of hidden attractors in such systems as well. In this case, the condition will be that the basin of attraction does not overlap with the fixed point that represents the basic switching cycle.

General information
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Organisations: Department of Physics, South West State University
Multistability, Hidden attractor, Multilevel DC/DC converter, High feedback gain, Border-collision bifurcations
Multistability and hidden attractors in an impulsive Goodwin oscillator with time delay

The release of luteinizing hormone (LH) is driven by intermittent bursts of activity in the hypothalamic nerve centers of the brain. Luteinizing hormone again stimulates release of the male sex hormone testosterone (Te) and, via the circulating concentration of Te, the hypothalamic nerve centers are subject to a negative feedback regulation that is capable of modifying the intermittent bursts into more regular pulse trains. Bifurcation analysis of a hybrid model that attempts to integrate the intermittent bursting activity with a continuous hormone secretion has recently demonstrated a number of interesting nonlinear dynamic phenomena, including bistability and deterministic chaos. The present paper focuses on the additional complexity that arises when the time delay in the continuous part of the model exceeds the typical bursting interval of the feedback. Under these conditions, the hybrid model is capable of displaying quasiperiodicity and border collisions as well as multistability and hidden attractors.

General information
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Organisations: Department of Physics, Southwest State University, St. Petersburg State University, Uppsala University
Authors: Zhusubaliyev, Z. T. (Ekstern), Mosekilde, E. (Intern), Churilov, A. N. (Ekstern), Medvedev, A. (Ekstern)
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BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.94 SJR 0.581 SNIP 0.817
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.642 SNIP 0.904 CiteScore 1.68
Web of Science (2015): Indexed yes
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BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.924 SNIP 0.773 CiteScore 1.44
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Multistability and hidden attractors in a relay system with hysteresis

For nonlinear dynamic systems with switching control, the concept of a "hidden attractor" naturally applies to a stable dynamic state that either (1) coexists with the stable switching cycle or (2), if the switching cycle is unstable, has a basin of attraction that does not intersect with the neighborhood of that cycle. We show how the equilibrium point of a relay system disappears in a boundary-equilibrium bifurcation as the system enters the region of autonomous switching dynamics and demonstrate experimentally how a relay system can exhibit large amplitude chaotic oscillations at high values of the supply voltage. By investigating a four-dimensional model of the experimental relay system we finally show how a variety of hidden periodic, quasiperiodic and chaotic attractors arise, transform and disappear through different bifurcations. (C) 2015 Elsevier B.V. All rights reserved.
Nanoporous gyroid TiO$_2$ and SnO$_2$ by melt infiltration of block copolymer templates

Abstract Fabrication of meso-porous metal oxide thin films with high surface area is a crucial requirement for numerous applications, such as catalysis, photovoltaics and electronics. Despite considerable progress in fabrication of three-dimensional metal oxide nanostructures, it is still quite challenging to manufacture highly ordered structures over a large area in a controlled way. The main objective of this study is to demonstrate fabrication of interconnected, crack-free and highly ordered ceramic films using a nano-porous polymer with gyroid morphology as template. Titanium tetraisopropoxide and tin chloride dihydrate are used as precursors for nanostructured TiO$_2$ and SnO$_2$, respectively. Complete precursor infiltration into the template and successful transformation into metal oxides can be achieved by rational tuning of the template chemistry. As a result, thin films of nanostructured metal oxides with gyroid morphology, such as titania and tin dioxide, are created and thoroughly characterized by scanning electron microscopy, transmission electron microscopy,
energy-dispersive analysis, x-ray diffraction and Brunauer-Emmett-Teller analysis.

**General information**

**State:** Published

**Organisations:** Department of Micro- and Nanotechnology, Self-organized Nanoporous Materials, Experimental Surface and Nanomaterials Physics, Silicon Microtechnology, Center for Nanostructured Graphene

**Authors:** Li, T. (Intern), Schulte, L. (Intern), Hansen, O. (Intern), Ndoni, S. (Intern)

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- Web of Science (2017): Indexed Yes
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- Web of Science (2016): Indexed yes
- BFI (2015): BFI-level 1
- Scopus rating (2015): SJR 1.184 SNIP 1.168 CiteScore 3.55
- Web of Science (2015): Indexed yes
- BFI (2014): BFI-level 1
- Scopus rating (2014): SJR 1.25 SNIP 1.282 CiteScore 3.55
- BFI (2013): BFI-level 1
- Scopus rating (2013): SJR 1.234 SNIP 1.354 CiteScore 3.39
- ISI indexed (2013): ISI indexed yes
- Web of Science (2013): Indexed yes
- BFI (2012): BFI-level 1
- Scopus rating (2012): SJR 1.496 SNIP 1.57 CiteScore 3.53
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- Web of Science (2012): Indexed yes
- BFI (2011): BFI-level 1
- Scopus rating (2011): SJR 1.524 SNIP 1.468 CiteScore 3.53
- ISI indexed (2011): ISI indexed yes
- Web of Science (2011): Indexed yes
- BFI (2010): BFI-level 1
- Scopus rating (2010): SJR 1.551 SNIP 1.403
- Web of Science (2010): Indexed yes
- BFI (2009): BFI-level 1
- Scopus rating (2009): SJR 1.25 SNIP 1.327
- BFI (2008): BFI-level 1
- Scopus rating (2008): SJR 1.373 SNIP 1.431
- Web of Science (2008): Indexed yes
- Scopus rating (2007): SJR 1.392 SNIP 1.418
- Web of Science (2007): Indexed yes
- Scopus rating (2006): SJR 1.51 SNIP 1.364
- Scopus rating (2005): SJR 1.408 SNIP 1.766
- Scopus rating (2004): SJR 1.344 SNIP 1.633
- Web of Science (2004): Indexed yes
Numerical modelling of the transition from low to high confinement in magnetically confined plasma

General information
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Organisations: Department of Physics, Plasma Physics and Fusion Energy, Chinese Academy of Sciences
Authors: Rasmussen, J. J. (Intern), Nielsen, A. H. (Intern), Madsen, J. (Intern), Naulin, V. (Intern), Xu, G. S. (Ekstern)
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Publication date: 2015
Main Research Area: Technical/natural sciences

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Observation of gliding arc surface treatment
An alternating current (AC) gliding arc can be conveniently operated at atmospheric pressure and efficiently elongated into the ambient air by an air flow and thus is useful for surface modification. A high speed camera was used to capture dynamics of the AC gliding arc in the presence of polymer surfaces. A gap was observed between the polymer surface and the luminous region of the plasma column, indicating the existence of a gas boundary layer. The thickness of the gas boundary layer is smaller at higher gas flow-rates or with ultrasonic irradiation to the AC gliding arc and the polymer surface. Water contact angle measurements indicate that the treatment uniformity improves significantly when the AC gliding arc is tilted to the polymer surface. Thickness reduction of the gas boundary layer, explaining the improvement of surface treatment, by the ultrasonic irradiation was directly observed for the first time.

General information
State: Published
Organisations: Department of Wind Energy, Composites and Materials Mechanics, Department of Physics, Plasma Physics and Fusion Energy, Lund University, Danish Technological Institute, FORCE Technology
Authors: Kusano, Y. (Intern), Zhu, J. (Ekstern), Ehn, A. (Ekstern), Li, Z. (Ekstern), Aldén, M. (Ekstern), Salewski, M. (Intern), Leipold, F. (Intern), Bardenshtein, A. (Ekstern), Krebs, N. (Ekstern)
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Observations of the effect of lower hybrid waves on ELM behaviour in EAST

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Organisations: Plasma Physics and Fusion Energy, Department of Physics, Chinese Academy of Sciences, University of Science and Technology of China
Authors: Chen, R. (Ekstern), Xu, G. (Ekstern), Liang, Y. (Ekstern), Wang, H. (Ekstern), Zhou, C. (Ekstern), Liu, A. (Ekstern), Wang, L. (Ekstern), Qian, J. (Ekstern), Gan, K. (Ekstern), Yang, J. (Ekstern), Duan, Y. (Ekstern), Li, Y. (Ekstern), Ding, S. (Ekstern), Wu, X. (Ekstern), Yan, N. (Intern), Chen, L. (Ekstern), Shao, L. (Ekstern), Zhang, W. (Ekstern), Hu, G.
On analytic continuability of the missing Cauchy datum for Helmholtz boundary problems

We relate the domains of analytic continuation of Dirichlet and Neumann boundary data for Helmholtz problems in two or more independent variables. The domains are related à priori, locally and explicitly in terms of complex polyrectangular neighbourhoods of planar pieces of the boundary. To this end we identify and characterise a special subspace of the standard pseudodifferential operators with real-analytic symbols. The result is applicable in the estimation of the domain of analytic continuation of solutions across planar pieces of the boundary.

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Authors: Karamehmedovic, M. (Intern)
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Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.282 SNIP 1.092 CiteScore 0.71
BFI (2013): BFI-level 1
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One-dimensional modelling of limit-cycle oscillation and H-mode power scaling

To understand the connection between the dynamics of microscopic turbulence and the macroscale power scaling in the L-I-H transition in magnetically confined plasmas, a new time-dependent, one-dimensional (in radius) model has been developed. The model investigates the radial force balance equation at the edge region of the plasma and applies the quenching effect of turbulence via the E x B flow shear rate exceeding the shear suppression threshold. By slightly ramping up the heating power, the spatio-temporal evolution of turbulence intensity, density and pressure profiles, poloidal flow and E x B flow selfconsistently displays the L-H transition with an intermediate phase (I-phase) characterized by limit-cycle oscillations. Since the poloidal flow is partially damped to the neoclassical flow in the edge region, the numerical results reveal two different oscillation relationships between the E x B flow and the turbulence intensity depending on which oscillation of the diamagnetic flow or poloidal flow is dominant. Specifically, by including the effects of boundary conditions of density and temperature, the model results in a linear dependence of the H-mode access power on the density and magnetic field. These results imply that the microscopic turbulence dynamics and the macroscale power scaling for the L-H transition are strongly connected.

One-dimensional modelling of limit-cycle oscillation and H-mode power scaling

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**General information**

State: Published

Organisations: Department of Physics, Plasma Physics and Fusion Energy, Chinese Academy of Sciences

Authors: Wu, X. (Ekstern), Xu, G. (Ekstern), Wan, B. (Ekstern), Juul Rasmussen, J. (Intern), Naulin, V. (Intern), Nielsen, A. H. (Intern)

Number of pages: 12

Pages: 053029

Publication date: 2015

Main Research Area: Technical/natural sciences

**Publication information**

Journal: Nuclear Fusion

Volume: 55
Onset of chaos in a single-phase power electronic inverter

Supported by experiments on a power electronic DC/AC converter, this paper considers an unusual transition from the domain of stable periodic dynamics (corresponding to the desired mode of operation) to chaotic dynamics. The behavior of the converter is studied by means of a 1D stroboscopic map derived from a non-autonomous ordinary differential equation with discontinuous right-hand side. By construction, this stroboscopic map has a high number of border points. It is shown that the onset of chaos occurs stepwise, via irregular cascades of different border collisions, some of which lead to bifurcations while others do not.

Publication information
Journal: Chaos
Volume: 25
Issue number: 4
Article number: 043114
ISSN (Print): 1054-1500
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 2.07 SJR 0.716 SNIP 0.829
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 1.76 SJR 0.78 SNIP 0.943
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.829 SNIP 1.005 CiteScore 1.76
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 0.94 SNIP 1.003 CiteScore 1.55
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 0.897 SNIP 0.956 CiteScore 1.5
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.078 SNIP 1.198 CiteScore 1.97
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.218 SNIP 1.071 CiteScore 1.98
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.508 SNIP 1.056
Web of Science (2010): Indexed yes
On the calculation of x-ray scattering signals from pairwise radial distribution functions

We derive a formulation for evaluating (time-resolved) x-ray scattering signals of solvated chemical systems, based on pairwise radial distribution functions, with the aim of this formulation to accompany molecular dynamics simulations. The derivation is described in detail to eliminate any possible ambiguities, and the result includes a modification to the atom-type formulation which to our knowledge is previously unaccounted for. The formulation is numerically implemented and validated.

General information

State: Published
Organisations: Center for Atomic-scale Materials Design, Department of Chemistry, Department of Physics, Neutrons and X-rays for Materials Physics, Physical and Biophysical Chemistry
Authors: Dohn, A. O. (Intern), Biasin, E. (Intern), Haldrup, K. (Intern), Nielsen, M. M. (Intern), Henriksen, N. E. (Intern), Møller, K. B. (Intern)
Number of pages: 9
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information

Journal: Journal of Physics B: Atomic, Molecular and Optical Physics
Volume: 48
Issue number: 24
Article number: 244010
ISSN (Print): 0953-4075
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): SNIP 0.884 SJR 0.85 CiteScore 1.77
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 1.22 SJR 0.781 SNIP 0.759
Web of Science (2016): Indexed yes
Crystals with a hexagonal close-packed (HCP) structure are inherently anisotropic, and have a limited number of independent slip systems, which leads to strong deformation textures and reduced formability in polycrystalline products. Tension along the c-axis of the crystal ideally activates extension twinning as a deformation mode due to the lack of easy-slip systems. In this work, experiments were devised to study extension twinning in a polycrystalline Mg alloy AZ31B with a strong basal rolling texture by tensile deformation parallel to the plate normal. Three-dimensional synchrotron X-ray diffraction (3DXRD) was used to map the center-of-mass positions, volumes, orientations, elastic strains, and stress tensors of over 1400 grains in-situ up to a true strain of 1.4%. More than 700 tensile twins were observed to form in the mapped volume under deformation. The measured center-of-mass positions and grain volumes are used to construct various 3D microstructures and model them with a Crystal Plasticity Finite Element (CPF) code. It is observed that the average grain-resolved stress did not always select the highest ranked Schmid factor twin variant. In fact, the contribution...
of lower ranked variants was non-negligible. The CPFE simulation indicates that there is a small variation in the stress within each grain in the elastic regime, which increases drastically upon the onset of plasticity. One of the significant outcomes of this work is the new statistical information on the interaction between twin and parent grain. It is shown that, on average, there is a small difference between the stress normal to the twin habit plane in the parent and twin, but that this is not the case for the shear acting on the habit plane.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, University of Oxford, Deutsches Elektronen-Synchrotron, Queen's University, University of Manchester
Authors: Abdolvand, H. (Ekstern), Majkut, M. (Intern), Oddershede, J. (Intern), Schmidt, S. (Intern), Lienert, U. (Ekstern), Diak, B. J. (Ekstern), Withers, P. J. (Ekstern), Daymond, M. R. (Ekstern)
Number of pages: 21
Pages: 77-97
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: International Journal of Plasticity
Volume: 70
ISSN (Print): 0749-6419
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): CiteScore 5.97 SJR 3.395 SNIP 2.752
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 5.84 SJR 3.691 SNIP 3.033
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 4.537 SNIP 3.062 CiteScore 6.07
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 5.259 SNIP 3.542 CiteScore 6.5
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 4.359 SNIP 3.441 CiteScore 6.41
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 3.914 SNIP 2.948 CiteScore 4.76
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 4.077 SNIP 2.985 CiteScore 5.08
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 5.223 SNIP 3.474
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 3.622 SNIP 2.617
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 4.047 SNIP 2.872
Web of Science (2008): Indexed yes
Web of Science (2007): Indexed yes
On the importance of sensor height variation for detection of magnetic labels by magnetoresistive sensors

Magnetoresistive sensors are widely used for biosensing by detecting the signal from magnetic labels bound to a functionalized area that usually covers the entire sensor structure. Magnetic labels magnetized by a homogeneous applied magnetic field weaken and strengthen the applied field when they are over and outside the sensor area, respectively, and the detailed origin of the sensor signal in experimental studies has not been clarified. We systematically analyze the signal from both a single sensor stripe and an array of sensor stripes as function of the geometrical parameters of the sensor stripes as well as the distribution of magnetic labels over the stripes. We show that the signal from sensor stripes with a uniform protective coating, contrary to conventional wisdom in the field, is usually dominated by the contribution from magnetic labels between the sensor stripes rather than by the labels on top of the sensor stripes because these are at a lower height. We therefore propose a shift of paradigm to maximize the signal due to magnetic labels between sensor stripes. Guidelines for this optimization are provided and illustrated for an experimental case from the literature.

General information
State: Published
Organisations: Department of Micro- and Nanotechnology, Magnetic Systems, Department of Physics, Stanford University
Authors: Henriksen, A. D. (Intern), Wang, S. X. (Ekstern), Hansen, M. F. (Intern)
Number of pages: 11
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Scientific Reports
Volume: 5
Article number: 12282
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
On the stability of copper overlayers on Au(1 1 1) and Au(1 0 0) electrodes under low potential conditions and in the presence of CO and CO2

We have studied the stability of Cu overlayers on Au(1 1 1) and Au(1 0 0) electrodes under low potential conditions and in the presence of CO and CO2 by means of electrochemical STM (EC-STM). For preparation we utilized the well known underpotential deposition (UPD) of copper, which, depending on the electrolyte (HClO4 and H2SO4), leads to Cu coverages in the submonolayer to monolayer range. For a Cu submonolayer on Au(1 1 1) we found that independent from the actual gas coadsorbate its closed film-like structure collapses at low potentials due to the desorption of coadsorbed anions. In contrast we found for a full Cu monolayer on Au(1 1 1) and Au(1 0 0) the formation of an alloy phase under low potential conditions, which also occurs independent from the presence of gas coadsorbates.
Optical laser-induced CO desorption from Ru(0001) monitored with a free-electron X-ray laser: DFT prediction and X-ray confirmation of a precursor state

We present density functional theory modeling of time-resolved optical pump/X-ray spectroscopic probe data of CO desorption from Ru(0001). The BEEF van der Waals functional predicts a weakly bound state as a precursor to desorption. The optical pump leads to a near-instantaneous (∼100 fs) increase of the electronic temperature to nearly 7000 K. The temperature evolution and energy transfer between electrons, substrate phonons and adsorbate is described by the two-temperature model and found to equilibrate on a timescale of a few picoseconds to an elevated local temperature of ∼2000 K. Estimating the free energy based on the computed potential of mean force along the desorption path, we find an entropic barrier to desorption (and by time-reversal also to adsorption). This entropic barrier separates the chemisorbed and precursor states, and becomes significant at the elevated temperature of the experiment (∼1.4 eV at 2000 K). Experimental pump-probe X-ray absorption/X-ray emission spectroscopy indicates population of a precursor state to desorption upon laser-excitation of the system (Dell'Angela et al., 2013). Computing spectra along the desorption path confirms the picture of a weakly bound transient state arising from ultrafast heating of the metal substrate.
Optical manipulation with two beam traps in microfluidic polymer systems

An optical trapping system with two opposing laser beams, also known as the optical stretcher, are naturally constructed inside a microfluidic lab-on-chip system. We present and compare two approaches to combine a simple microfluidic system with either waveguides directly written in the microfluidic chip or with optical fibers mounted in the chip.

General information
State: Published
Organisations: Department of Physics, Department of Micro- and Nanotechnology, Optofluidics, Biophysics and Fluids, NIL Technology ApS
Authors: Khoury Arvelo, M. (Intern), Matteucci, M. (Intern), Sørensen, K. T. (Intern), Bilenberg, B. (Ekstern), Vannahme, C. (Intern), Kristensen, A. (Intern), Berg-Sørensen, K. (Intern)
Number of pages: 2
Publication date: 2015

Host publication information
Title of host publication: 2015 20th Microoptics Conference (MOC)
Publisher: IEEE
ISBN (Print): 978-4-8634-8487-0
Main Research Area: Technical/natural sciences
Conference: 20th Microoptics Conference, Fukuoka, Japan, 25/10/2015 - 25/10/2015
DOIs: 10.1109/MOC.2015.7416377
Source: FindIt
Source-ID: 277283421
Publication: Research - peer-review › Article in proceedings – Annual report year: 2016

Optical properties of photovoltaic Cu$_2$SnS$_3$ films deposited on soda lime glass and Mo-coated glass

General information
State: Published
Organisations: Department of Micro- and Nanotechnology, Silicon Microtechnology, Department of Photonics Engineering, Optical Microsensors and Micromaterials, Department of Physics, Experimental Surface and Nanomaterials Physics
Authors: Crovetto, A. (Intern), Ettlinger, R. B. (Intern), Schou, J. (Intern), Hansen, O. (Intern)
Number of pages: 1
Publication date: 2015
Main Research Area: Technical/natural sciences
Electronic versions: ancro_Poster_EMRS_2015.pdf
Optical properties of pulsed laser-deposited \( \text{Cu}_2\text{SnS}_3 \) films for photovoltaics

**General information**

**State:** Published

**Organisations:** Department of Micro- and Nanotechnology, Silicon Microtechnology, Department of Photonics Engineering, Optical Microsensors and Micromaterials, Department of Physics, Experimental Surface and Nanomaterials Physics

**Authors:** Crovetto, A. (Intern), Ettlinger, R. B. (Intern), Schou, J. (Intern), Hansen, O. (Intern)

**Number of pages:** 1

**Publication date:** 2015

**Host publication information**

**Title of host publication:** Book of abstracts : EMRS 2015 Spring meeting

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

**Conference:** European Materials Research Society (E-MRS) Spring Meeting 2015, Lille, France, 11/05/2015 - 11/05/2015

**Electronic versions:**

ancro_abstract_EMRS_spring_2015.pdf

**Source:** PublicationPreSubmission

**Source-ID:** 114603229

**Publication:** Research - peer-review › Conference abstract in proceedings – Annual report year: 2015

Optimal Design of Silicon-based Chips for Piezo-induced Ultrasound Resonances in Embedded Microchannels

We present a variational formulation of the governing equations and introduce global indicators to describe the behavior of acoustofluidic devices driven at resonance frequencies by means of a piezoelectric transducer. The individuation of the correct Lagrangian densities for the different parts constituting the device (the piezo transducer, the silicon walls, the fluid-filled microchannel, and the glass lid) allows for the introduction of the weak formulation used in the finite element discretization of the equations describing the system in its oscillatory regime. Additionally, the knowledge of the Lagrangian density leads to the derivation of the correct structure of the Hamiltonian density, i.e. the energy density, which is important for the quantification of the energy content of the whole system and its individual parts. Specifically, the energy content of the embedded microchannel is quantified by means of the acoustofluidic yield $\eta$ defined as the ratio between the energy in the channel and the total energy. From the standpoint of acoustophoretic application, the introduction of the acoustophoretic mean orientation allows us to identify the frequencies for which an acoustophoretic effect, i.e. the lateral motion of particle dragged by the axial main flow, is particularly strong. Finally, the connection between the mechanical and electrical degrees of freedom of the system is addressed. This is important for proper determination of the dissipated power, and it may lead to the detection of resonance states by means of purely electrical measurements. Numerical simulations and preliminary experimental results show some features of the model introduced.

**General information**

**State:** Published

**Organisations:** Department of Physics, Biophysics and Fluids, Lund University

**Authors:** Garofalo, F. (Ekstern), Laurell, T. (Ekstern), Bruus, H. (Intern)

**Pages:** 50-54

**Publication date:** 2015

**Conference:** 2015 International Congress on Ultrasonics, Metz, France, 10/05/2015 - 10/05/2015

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

**Publication information**

**Journal:** Physics Procedia

**Volume:** 70

**ISSN (Print):** 1875-3892

**Ratings:**

Scopus rating (2017): SNIP 0.614 SJR 0.351 CiteScore 0.67

Scopus rating (2016): CiteScore 0.65 SJR 0.347 SNIP 0.574

Scopus rating (2015): SJR 0.262 SNIP 0.572 CiteScore 0.61

Scopus rating (2014): SJR 0.401 SNIP 0.696 CiteScore 0.78

Scopus rating (2013): SJR 0.29 SNIP 0.605 CiteScore 0.72

ISI indexed (2013): ISI indexed no

Scopus rating (2012): SJR 0.28 SNIP 0.623 CiteScore 0.5

ISI indexed (2012): ISI indexed no
Optimizing shape uniformity and increasing structure heights of deep reactive ion etched silicon x-ray lenses: Paper

Line-focusing compound silicon x-ray lenses with structure heights exceeding 300 μm were fabricated using deep reactive ion etching. To ensure profile uniformity over the full height, a new strategy was developed in which the perimeter of the structures was defined by trenches of constant width. The remaining sacrificial material inside the lens cavities was removed by etching through the silicon wafer. Since the wafers become fragile after through-etching, they were then adhesively bonded to a carrier wafer. Individual chips were separated using laser micro machining and the 3D shape of fabricated lenses was thoroughly characterized by a variety of means. Optical testing using synchrotron radiation with a photon energy of 58 keV yielded a 300 μm wide beam with a waist of 980 nm (full width at half maximum) at a focal length of 1.3 m. Optical aberrations are discussed in the context of the shape analysis, where a slight bowing of the lens sidewalls and an insufficiently uniform apex region are identified as resolution-limiting factors. Despite these, the proposed fabrication route proved a viable approach for producing x-ray lenses with large structure heights and provides the means to improve the resolution and capabilities of modern x-ray techniques such as x-ray microscopy and 3D x-ray diffraction.

General information
State: Published
Organisations: DTU Danchip, Department of Physics, Neutrons and X-rays for Materials Physics, Experimental Surface and Nanomaterials Physics, Department of Micro- and Nanotechnology, Silicon Microtechnology, European Synchrotron Radiation Facility
Authors: Stöhr, F. (Intern), Wright, J. (Ekstern), Simons, H. (Intern), Michael-Lindhard, J. (Intern), Hübner, J. (Intern), Jensen, F. (Intern), Hansen, O. (Intern), Poulsen, H. F. (Intern)
Number of pages: 10
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Micromechanics and Microengineering
Volume: 25
Issue number: 12
Article number: 125013
ISSN (Print): 0960-1317
Ratings:
Web of Science (2018): Indexed yes
BFI (2018): BFI-level 1
Scopus rating (2017): SNIP 0.968 SJR 0.554 CiteScore 2.02
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.74 SJR 0.63 SNIP 1.067
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.687 SNIP 1.265 CiteScore 1.96
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.802 SNIP 1.316 CiteScore 1.84
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.737 SNIP 1.233 CiteScore 1.74
Overview of the JET results
Since the installation of an ITER-like wall, the JET programme has focused on the consolidation of ITER design choices and the preparation for ITER operation, with a specific emphasis given to the bulk tungsten melt experiment, which has been crucial for the final decision on the material choice for the day-one tungsten divertor in ITER. Integrated scenarios have been progressed with the re-establishment of long-pulse, high-confinement H-modes by optimizing the magnetic configuration and the use of ICRH to avoid tungsten impurity accumulation. Stationary discharges with detached divertor conditions and small edge localized modes have been demonstrated by nitrogen seeding. The differences in confinement and pedestal behaviour before and after the ITER-like wall installation have been better characterized towards the development of high fusion yield scenarios in DT. Post-mortem analyses of the plasma-facing components have confirmed the previously reported low fuel retention obtained by gas balance and shown that the pattern of deposition within the divertor has changed significantly with respect to the JET carbon wall campaigns due to the absence of thermally activated chemical erosion of beryllium in contrast to carbon. Transport to remote areas is almost absent and two orders of magnitude less material is found in the divertor.
Oxygen evolution on well-characterized mass-selected Ru and RuO$_2$ nanoparticles

Oxygen evolution was investigated on model, mass-selected RuO$_2$ nanoparticles in acid, prepared by magnetron sputtering. Our investigations include electrochemical measurements, electron microscopy, scanning tunneling microscopy and X-ray photoelectron spectroscopy. We show that the stability and activity of nanoparticulate RuO$_2$ is highly sensitive to its surface pretreatment. At 0.25 V overpotential, the catalysts show a mass activity of up to 0.6 A mg$^{-1}$ and a turnover frequency of 0.65 s$^{-1}$, one order of magnitude higher than the current state-of-the-art.
Oxygen reduction on nanocrystalline ruthenia-local structure effects

Nanocrystalline ruthenium dioxide and doped ruthenium of the composition Ru1-xMxO2 (M = Co, Ni, Zn) with 0 ≤ x ≤ 0.2 were prepared by the spray-freezing freeze-drying technique. The oxygen reduction activity and selectivity of the prepared materials were evaluated in alkaline media using the RRDE methodology. All ruthenium based oxides show a strong preference for a 2-electron oxygen reduction pathway at low overpotentials. The catalysts' selectivity shifts towards the 4-electron reduction pathway at high overpotentials (i.e. at potentials below 0.4 V vs. RHE). This trend is particularly noticeable on non-doped and Zn-doped catalysts; the materials containing Ni and Co produce a significant fraction of hydrogen peroxide even at high overpotentials. The suppression of the 4-electron reduction pathway on Ni and Co-doped catalysts can be accounted for by the presence of the Ni and Co cations in the cus binding sites as shown by the DFT-based analyses on non-doped and doped catalysts.
Particle source and edge transport studies in JET H-mode gas puff modulation experiments

General information
State: Published
Organisations: Department of Physics, Plasma Physics and Fusion Energy, VTT - Technical Research Centre of Finland, Istituto di Fisica del Plasma, Aalto University, Universidade de Lisboa, College of William and Mary, IPP, European Fusion Development Agreement, Culham Science Centre, Centre de Recherches en Physique des Plasmas
Authors: Salmi, A. (Ekstern), Tala, T. (Ekstern), Mantica, P. (Ekstern), Järvinen, A. (Ekstern), Meneses, L. (Ekstern), Mordjick, S. (Ekstern), Naulin, V. (Intern), Rasmussen, J. J. (Intern), Svensson, J. (Ekstern), Giacomelli, L. (Ekstern), Gomes, R. (Ekstern), Groth, M. (Ekstern), Koskela, T. (Ekstern), Maggi, C. (Ekstern), Maslov, M. (Ekstern), Sips, G. (Ekstern), Weisen, H. (Ekstern)
Number of pages: 4
Publication date: 2015
Main Research Area: Technical/natural sciences
Source: FindIt
Source-ID: 273336118
Publication: Research - peer-review › Journal article – Annual report year: 2014

Photocatalytic Water Splitting: Using a 2-Photon Tandem Approach

General information
State: Published
Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics, Department of Micro- and Nanotechnology, Silicon Microtechnology, Aalto University
Authors: Seger, B. (Intern), Mei, B. T. (Intern), Bae, D. (Intern), Kemppainen, E. (Ekstern), Pedersen, T. (Intern), Vesborg, P. (Intern), Hansen, O. (Intern), Chorkendorff, I. (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-1
Main Research Area: Technical/natural sciences
Conference: DTU Sustain Conference 2015, Lyngby, Denmark, 17/12/2015 - 17/12/2015
Electronic versions:
E1_DTU_Sustain_2015.pdf
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2015
Physical properties of the GaPd₂ intermetallic catalyst in bulk and nanoparticle morphology

Intermetallic compound GaPd₂ is a highly selective catalyst material for the semi-hydrogenation of acetylene. We have determined anisotropic electronic, thermal and magnetic properties of a GaPd₂ monocrystal along three orthogonal orthorhombic directions of the structure. By using ⁶⁹Ga and ⁷¹Ga NMR spectroscopy, we have determined the electric-field-gradient tensor at the Ga site in the unit cell and the Knight shift, which yields the electronic density of states (DOS) at the Fermi energy ε₉. The DOS at ε₉ was determined independently also from the specific heat. To see the change of electronic properties of the GaPd₂ phase on going from the bulk material to the nanoparticles morphology, we have synthesized GaPd₂/SiO₂ supported nanoparticles and determined their electronic DOS at ε₉ from the ⁷¹Ga NMR spin-lattice relaxation rate. The electronic DOS of the GaPd₂ was also studied theoretically from first principles. All results are compared to the chemically related compound GaPd. The active-site-isolation concept for an increased catalytic selectivity is discussed in relation to the GaPd₂ and GaPd structures.
Plasma rotation and ion temperature measurements by collective Thomson scattering at ASDEX Upgrade

We present the first deuterium ion temperature and rotation measurements by collective Thomson scattering at ASDEX Upgrade. The results are in general agreement with boron-based charge exchange recombination spectroscopy measurements and consistent with neoclassical simulations for the plasma scenario studied here. This demonstration opens the prospect for direct non-perturbative measurements of the properties of the main ion species in the plasma core with applications in plasma transport and confinement studies.

General information
State: Published
Organisations: Department of Physics, Plasma Physics and Fusion Energy, Max-Planck-Institut für Plasmaphysik
Number of pages: 1
Pages: 062001
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Plasma Physics and Controlled Fusion
Volume: 57
Issue number: 6
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Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 1.243 SJR 0.69 CiteScore 1.74
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1 SJR 1.433 SNIP 1.258
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.314 SNIP 1.345 CiteScore 1.1
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.542 SNIP 1.346 CiteScore 1.61
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.2 SNIP 1.253 CiteScore 1.54
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.453 SNIP 1.201 CiteScore 1.63
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.496 SNIP 1.591 CiteScore 2.69
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Plasma transport in the Scrape-off-Layer of magnetically confined plasma and the plasma exhaust

An overview of the plasma dynamics in the Scrape-off-Layer (SOL) of magnetically confined plasma is presented. The SOL is the exhaust channel of the warm plasma from the core, and the understanding of the SOL plasma dynamics is one of the key issues in contemporary fusion research. It is essential for operation of fusion experiments and ultimately fusion power plants. Recent results clearly demonstrate that the plasma transport through the SOL is dominated by turbulent intermittent fluctuations organized into filamentary structures convecting particles, energy, and momentum through the SOL region. Thus, the transport cannot be described and parametrized by simple diffusive type models. The transport leads to strong localized power loads on the first wall and the plasma facing components, which have serious lasting influence.

General information
State: Published
Organisations: Department of Physics, Plasma Physics and Fusion Energy, Technical University of Denmark, UiT The Arctic University of Norway, University of Innsbruck, Ecole Polytechnique Federale de Lausanne (EPFL), Chinese Academy of Sciences
Authors: Rasmussen, J. J. (Intern), Naulin, V. (Intern), Nielsen, A. H. (Intern), Madsen, J. (Intern), Tophøj, L. E. H. (Intern), Christensen, A. (Ekstern), Magnusen, M. L. (Intern), Garcia, O. (Ekstern), Schmittwieser, R. (Ekstern), Ionita, C. (Ekstern), Costea, S. (Ekstern), Schneider, B. (Ekstern), Vianello, N. (Ekstern), Yan, N. (Ekstern), Xu, G. (Ekstern)
Number of pages: 4
Publication date: 2015
Main Research Area: Technical/natural sciences
Electronic versions:
J_J_Rasmussen_Topical_Review.pdf
Source: PublicationPreSubmission
Source-ID: 127770034
Publication: Research - peer-review › Paper – Annual report year: 2016
Plasmonic eigenmodes in individual and bow-tie graphene nanotriangles

In classical electrodynamics, nanostructured graphene is commonly modeled by the computationally demanding problem of a three-dimensional conducting film of atomic-scale thickness. Here, we propose an efficient alternative two-dimensional electrostatic approach where all calculation procedures are restricted to the graphene sheet. Furthermore, to explore possible quantum effects, we perform tight-binding calculations, adopting a random-phase approximation. We investigate multiple plasmon modes in 20 nm equilateral triangles of graphene, treating the optical response classically as well as quantum mechanically. Compared to the classical plasmonic spectrum which is "blind" to the edge termination, we find that the quantum plasmon frequencies exhibit blueshifts in the case of armchair edge termination of the underlying atomic lattice, while redshifts are found for zigzag edges. Furthermore, we find spectral features in the zigzag case which are associated with electronic edge states not present for armchair termination. Merging pairs of triangles into dimers, plasmon hybridization leads to energy splitting that appears strongest in classical calculations while splitting is lower for armchair edges and even more reduced for zigzag edges. Our various results illustrate a surprising phenomenon: Even 20 nm large graphene structures clearly exhibit quantum plasmonic features due to atomic-scale details in the edge termination.
Polarized neutron powder diffraction studies of antiferromagnetic order in bulk and nanoparticle NiO

In many materials it remains a challenge to reveal the nature of magnetic correlations, including antiferromagnetism and spin disorder. Revealing the spin structure in magnetic nanoparticles is further complicated by the large incoherent neutron scattering cross section from water adsorbed at the particle surfaces and by the broadening of diffraction peaks due to the finite crystallite size. Moreover, the spin structure in magnetic nanoparticles may deviate significantly from that of the corresponding bulk material because of the low-symmetry surroundings of surface atoms and the large relative surface contribution to the magnetic anisotropy. Here we explore the potential use of polarized neutron diffraction to reveal the magnetic structure in NiO bulk and nanoparticle powders by applying the XYZ-polarization analysis method. Our investigations address in particular the spin orientation in bulk NiO and platelet-shaped NiO nanoparticles with thickness from greater than 200 nm down to 2.0 nm. The advantage of the applied method is that it is able to clearly separate the structural, the magnetic, and the spin-incoherent scattering signals for all particle sizes. For platelet-shaped particles with thickness from greater than 200 nm down to 2.2 nm we find that the spin orientation deviates about 16° from the primary (111) plane of the platelet-shaped particles. In the smallest particles (2.0 nm thick) we find the spins are oriented with a 30° average angle to the primary (111) plane of the particles. The results show that polarization analyzed neutron powder diffraction is a viable method to investigate magnetic order in powders of antiferromagnetic nanoparticles.
We report on the structural and colorimetric effects of interaction of aqueous ∼0.06–1% poly[9,9-bis(2-ethylhexyl)fluorene]-
b-poly[3-6-trimethylammoniumhexyl]thiophene] bromide (PF2/6-P3TMAHT) with double-stranded DNA to form PF2/6-
P3TMAHT(DNA)x where x is the molar ratio of DNA base pairs to P3TMAHT repeat units; x = 0.5 equals the nominal charge neutralization. PF2/6-P3TMAHT forms 20–40 nm sized particles with PF2/6 core and hydrated P3TMAHT exterior. The polymer particles form loose one-dimensional chains giving micrometer long branched chains (0.19 ≤ x ≤ 0.76) and subsequently randomly shaped aggregates (x = 1.89) upon DNA addition. Compaction of the P3TMAHT block and the 20–30 nm sized core is observed for x = 0.38–0.76 and attributed to the DNA merged within P3TMAHT domain with this structure disassembling with DNA excess. Structural transformations are followed by chromic changes seen as color changes from deep red (x < 0.076) to yellow (x = 0.19), nearly colorless (x = 0.38–0.76), and back to orange (x = 1.89). Both absorption and photoluminescence spectra display the distinct fluorene and thiophene bands and subsequent blue and red shifts when passing x = 0.5. Thiophene photoluminescence (PL) is significantly quenched by DNA with increasing x, and the changing P3TMAHT/PF2/6 band ratio allows quantitative DNA detection. Sixteen-fold dilution does not change aggregate structure, but PL is blue-shifted, indicating weakened intermolecular interactions.

Polyelectrolyte Complexes of a Cationic All Conjugated Fluorene Thiophene Diblock Copolymer with Aqueous DNA

We report on the structural and colorimetric effects of interaction of aqueous ∼0.06–1% poly[9,9-bis(2-ethylhexyl)fluorene]-
b-poly[3-6-trimethylammoniumhexyl]thiophene] bromide (PF2/6-P3TMAHT) with double-stranded DNA to form PF2/6-
P3TMAHT(DNA)x where x is the molar ratio of DNA base pairs to P3TMAHT repeat units; x = 0.5 equals the nominal charge neutralization. PF2/6-P3TMAHT forms 20–40 nm sized particles with PF2/6 core and hydrated P3TMAHT exterior. The polymer particles form loose one-dimensional chains giving micrometer long branched chains (0.19 ≤ x ≤ 0.76) and subsequently randomly shaped aggregates (x = 1.89) upon DNA addition. Compaction of the P3TMAHT block and the 20–30 nm sized core is observed for x = 0.38–0.76 and attributed to the DNA merged within P3TMAHT domain with this structure disassembling with DNA excess. Structural transformations are followed by chromic changes seen as color changes from deep red (x < 0.076) to yellow (x = 0.19), nearly colorless (x = 0.38–0.76), and back to orange (x = 1.89). Both absorption and photoluminescence spectra display the distinct fluorene and thiophene bands and subsequent blue and red shifts when passing x = 0.5. Thiophene photoluminescence (PL) is significantly quenched by DNA with increasing x, and the changing P3TMAHT/PF2/6 band ratio allows quantitative DNA detection. Sixteen-fold dilution does not change aggregate structure, but PL is blue-shifted, indicating weakened intermolecular interactions.

General information

State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Helmholtz-Zentrum Geesthacht: Zentrum für Material- und Küstenforschung GmbH, University of Bayreuth, University of Wuppertal, University of Coimbra
Authors: Knaapila, M. (Intern), Costa, T. (Ekstern), Garamus, V. M. (Ekstern), Kraft, M. (Ekstern), Drechsler, M. (Ekstern), Scherf, U. (Ekstern), Burrows, H. D. (Ekstern)
Number of pages: 11
Pages: 3231-3241
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Polymer injection molding of hard X-ray refractive optics

General information
State: Published
Organisations: DTU Danchip, Neutrons and X-rays for Materials Physics, Department of Physics, Experimental Surface and Nanomaterials Physics, Department of Micro- and Nanotechnology, Silicon Microtechnology
Number of pages: 1
Publication date: 2015
Main Research Area: Technical/natural sciences
X-ray optics, Polymer injection molding, Deep reactive ion etching
Electronic versions:
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Source-ID: 118322738
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2015

Prediction of beam hardening artefacts in computed tomography using Monte Carlo simulations

We show how radiological images of both single and multi material samples can be simulated using the Monte Carlo simulation tool McXtrace and how these images can be used to make a three dimensional reconstruction. Good numerical agreement between the X-ray attenuation coefficient in experimental and simulated data can be obtained, which allows us to use simulated projections in the linearisation procedure for single material samples and in that way reduce beam hardening artefacts. The simulations can be used to predict beam hardening artefacts in multi material samples with complex geometry, illustrated with an example. Linearisation requires knowledge about the X-ray transmission at varying sample thickness, but in some cases homogeneous calibration phantoms are hard to manufacture, which affects the accuracy of the calibration. Using simulated data overcomes the manufacturing problems and in that way improves the calibration. (C) 2014 Elsevier B.V. All rights reserved.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, University of Copenhagen, Lund University, Technical University of Munich, University of Munich, Novo Nordisk A/S
Authors: Thomsen, M. (Ekstern), Bergbäck Knudsen, E. (Intern), Willendrup, P. K. (Intern), Bech, M. (Ekstern), Willner, M. (Ekstern), Pfeiffer, F. (Ekstern), Poulsen, M. (Ekstern), Løffmann, K. (Ekstern), Feidenhans'l, R. (Ekstern)
Number of pages: 7
Pages: 314-320
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Main Research Area: Technical/natural sciences

Publication information
Journal: Nuclear Instruments and Methods in Physics Research Section B: Beam Interactions with Materials and Atoms
Volume: 342
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 1.02 SJR 0.558 CiteScore 1.36
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
We discuss recent developments for studying plasmonic metal nanostructures. Exploiting photons and electrons opens up new capabilities to probe the complete plasmon spectrum including bright and dark modes and related local optical fields at subnanometer spatial resolution. This comprehensive characterization of plasmonic properties of metal nanostructures provides new basic insight into the fundamental physics of "surface enhanced" spectroscopy in hottest hot spots and
enables us to optimize plasmon supported processes and devices.

**General information**
- **State:** Published
- **Organisations:** Department of Physics, Biophysics and Fluids, Humboldt-University of Berlin
- **Authors:** Kneipp, K. (Intern), Kneipp, H. (Intern), Kneipp, J. (Ekstern)
- **Number of pages:** 5
- **Pages:** 2721-2726
- **Publication date:** 2015
- **Main Research Area:** Technical/natural sciences

**Publication information**
- **Journal:** Chemical Science
- **Volume:** 6
- **Issue number:** 5
- **ISSN (Print):** 2041-6520
- **Ratings:**
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  - Web of Science (2018): Indexed yes
  - Scopus rating (2017): SNIP 1.666 SJR 4.508 CiteScore 8.54
  - Web of Science (2017): Indexed yes
  - BFI (2016): BFI-level 1
  - Scopus rating (2016): CiteScore 8.44 SJR 4.516 SNIP 1.659
  - BFI (2015): BFI-level 1
  - Web of Science (2015): Indexed yes
  - BFI (2014): BFI-level 1
  - Scopus rating (2014): SJR 4.995 SNIP 1.738 CiteScore 8.99
  - BFI (2013): BFI-level 1
  - Scopus rating (2013): SJR 4.698 SNIP 1.591 CiteScore 8.44
  - ISI indexed (2013): ISI indexed yes
  - Web of Science (2013): Indexed yes
  - BFI (2012): BFI-level 1
  - Scopus rating (2012): SJR 5.217 SNIP 1.829 CiteScore 8.18
  - ISI indexed (2012): ISI indexed yes
  - BFI (2011): BFI-level 1
  - Scopus rating (2011): SJR 4.362 SNIP 1.784 CiteScore 7.01
  - ISI indexed (2011): ISI indexed no
  - Web of Science (2011): Indexed yes
- **Original language:** English

**Chemistry, Enhanced raman-scattering, Single-molecule fluoresces, Local optical-fields, Fractal clusters, Metallic nanostructures, Nanoparticle dimers, Spectroscopy, Modes, Microscopy, Resonance, Nanostructures, Photons, Fundamental physics, Metal nanostructure, Optical field, Plasmon spectrum, Plasmonic nanostructures, Plasmonic properties, Spatial resolution, Sub nanometers, Plasmons**

**Electronic versions:**
- Probing_plasmonic_nanostructures_by_photons_and_electrons.pdf
- DOIs:
  - 10.1039/c4sc03508a
- Source: FindIt
- Source-ID: 274756574
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**Probing the Active Surface Sites for CO Reduction on Oxide-Derived Copper Electro catalysts**

CO electroreduction activity on oxide-derived Cu (OD-Cu) was found to correlate with metastable surface features that bind CO strongly. OD-Cu electrodes prepared by H-2 reduction of Cu2O precursors reduce CO to acetate and ethanol with nearly 50% Faradaic efficiency at moderate overpotential. Temperature-programmed desorption of CO on OD-Cu revealed the presence of surface sites with strong CO binding that are distinct from the terraces and stepped sites found on polycrystalline Cu foil. After annealing at 350 degrees C, the surface-area corrected current density for CO reduction is 44-fold lower and the Faradaic efficiency is less than 5%. These changes are accompanied by a reduction in the
proportion of strong CO binding sites. We propose that the active sites for CO reduction on OD-Cu surfaces are strong CO binding sites that are supported by grain boundaries. Uncovering these sites is a first step toward understanding the surface chemistry necessary for efficient CO electroreduction.

General information
State: Published
Organisations: Department of Physics, Center for Individual Nanoparticle Functionality, Stanford University, Technical University of Denmark, Lawrence Livermore National Laboratory
Authors: Verdaguer Casadevall, A. (Intern), Li, C. W. (Ekstern), Johansson, T. P. (Intern), Scott, S. B. (Ekstern), McKeown, J. T. (Ekstern), Kumar, M. (Ekstern), Stephens, I. E. L. (Intern), Kanan, M. W. (Ekstern), Chorkendorff, I. (Intern)
Number of pages: 4
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Main Research Area: Technical/natural sciences

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Journal: Journal of the American Chemical Society
Volume: 137
Issue number: 31
ISSN (Print): 0002-7863
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): SNIP 2.641 SJR 8.127 CiteScore 14.05
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 13.18 SJR 7.492 SNIP 2.596
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 6.775 SNIP 2.63 CiteScore 12.81
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 6.294 SNIP 2.587 CiteScore 11.92
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 5.993 SNIP 2.466 CiteScore 11.38
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 6.211 SNIP 2.38 CiteScore 10.37
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 5.478 SNIP 2.321 CiteScore 9.94
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 5.167 SNIP 2.138
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 5.06 SNIP 2.16
Web of Science (2008): Indexed yes
Protected methylammonium lead halide perovskite photoelectrodes for efficient two-photon water splitting

General information
State: Published
Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics
Authors: Bækbo, M. J. (Intern), Mei, B. T. (Intern), Bae, D. (Intern), Seger, B. (Intern), Vesborg, P. C. K. (Intern), Chorkendorff, I. (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-16
Main Research Area: Technical/natural sciences
Conference: DTU Sustain Conference 2015, Lyngby, Denmark, 17/12/2015 - 17/12/2015
Electronic versions:
E16_DTU_Sustain_2015.pdf

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Poster presentation
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2015

Pt-based catalysts for diesel exhaust oxidation: support effect and bimetallic elements

General information
State: Published
Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics, Center for Electron Nanoscopy, Technical University of Denmark
Authors: Silva, H. (Intern), Mazantti, N. (Ekstern), Spiga, C. (Intern), Chorkendorff, I. (Intern), Chakraborty, D. (Intern)
Number of pages: 1
Publication date: 2015

Host publication information
Title of host publication: Book of Abstracts. DTU's Sustain Conference 2015
Quantification of the impact of large and small-scale instabilities on the fast-ion confinement in ASDEX Upgrade

The confinement fast ions, generated by neutral beam injection (NBI), has been investigated at the ASDEX Upgrade tokamak. In plasmas that exhibit strong sawtooth crashes, a significant sawtooth-induced internal redistribution of mainly passing fast ions is observed, which is in very good agreement with the theoretical predictions based on the Kadomtsev model. Between the sawtooth crashes, the fishbone modes are excited which, however, do not cause measurable changes in the global fast-ion population. During experiments with on- and off-axis NBI and without strong magnetohydrodynamic (MHD) modes, the fast-ion measurements agree very well with the neo-classical predictions. This shows that the MHD-induced (large-scale), as well as a possible turbulence-induced (small-scale) fast-ion transport is negligible under these conditions. However, in discharges performed to study the off-axis NBI current drive efficiency with up to 10 MW of heating power, the fast-ion measurements agree best with the theoretical predictions that assume a weak level anomalous fast-ion transport. This is also in agreement with measurements of the internal inductance, a Motional Stark Effect diagnostic and a novel polarimetry diagnostic: the fast-ion driven current profile is clearly modified when changing the NBI injection geometry and the measurements agree best with the predictions that assume weak anomalous fast-ion diffusion.

General information
State: Published
Organisations: Department of Physics, Plasma Physics and Fusion Energy, Max Planck Institute, University of Seville
Number of pages: 15
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Publication date: 2015
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Publication Information
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Volume: 57
Issue number: 1
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 1.243 SJR 0.69 CiteScore 1.74
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1 SJR 1.433 SNIP 1.258
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.314 SNIP 1.345 CiteScore 1.1
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.542 SNIP 1.346 CiteScore 1.61
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.2 SNIP 1.253 CiteScore 1.54
A method for the extension of the three-dimensional X-ray diffraction technique to allow the extraction of domain volume fractions in polycrystalline ferroic materials is presented. This method gives access to quantitative domain volume fractions of hundreds of independent embedded grains within a bulk sample. Such information is critical to furthering our understanding of the grainscale interactions of ferroic domains and their influence on bulk properties. The method also provides a validation tool for mesoscopic ferroic domain modelling efforts. The mathematical formulations presented here are applied to tetragonal coarse-grained Ba$_{0.88}$Ca$_{0.12}$Zr$_{0.06}$Ti$_{0.94}$O$_3$ and rhombohedral fine-grained (0.82)Bi$_{0.5}$Na$_{0.5}$TiO$_3$–(0.18)Bi$_{0.5}$K$_{0.5}$TiO$_3$ electroceramic materials. The fitted volume fraction information is used to calculate grain-scale non-180° ferroelectric domain switching strains. The absolute errors are found to be approximately 0.01 and 0.03% for the tetragonal and rhombohedral cases, which had maximum theoretical domain switching strains of 0.47 and 0.54%, respectively. Limitations and possible extensions of the technique are discussed.
Quantum cryptography with an ideal local relay

We consider two remote parties connected to a relay by two quantum channels. To generate a secret key, they transmit coherent states to the relay, where the states are subject to a continuous-variable (CV) Bell detection. We study the ideal case where Alice's channel is lossless, i.e., the relay is locally in her lab and the Bell detection is performed with unit efficiency. This configuration allows us to explore the optimal performances achievable by CV measurement-device-independent quantum key distribution. This corresponds to the limit of a trusted local relay, where the detection loss can be re-scaled. Our theoretical analysis is confirmed by an experimental simulation where $10^{-4}$ secret bits per use can potentially be distributed at 170 km assuming ideal reconciliation.
Quantum theory of plasmons in nanostructures

In this thesis, \textit{ab initio} quantum-mechanical calculations are used to study the properties of plasmons in nanostructures that involve atomic length-scales. The plasmon is an electronic excitation that corresponds to oscillations in the electron charge density in metals, often visualized as water ripples in a pond where the water represents a sea of free electrons. Plasmons on metal surfaces and in nanostructured materials, such as metal nanoparticles and atomically thin two-dimensional materials, have several technological applications due to their ability to confine light on nanoscale. For a theoretical description of plasmon in such materials, where the electrons are heavily confined in one or more directions, a quantum mechanical description of the electrons in the material is necessary. In this thesis, the \textit{ab initio} methods Density functional theory (DFT) and linear response time-dependent DFT are applied to calculate the properties of plasmons in nanostructures in different dimensions. In order to identify and visualize localized plasmon modes, a method for calculating plasmon eigenmodes within the \textit{ab initio} framework has been developed. In the studied materials, quantum mechanical effects such as coupling to single-electronic transitions, electron spill-out from the surface, tunneling, and spatial non-locality, are shown to alter the plasmon excitations. The studied systems include two-dimensional materials, such as thin metal films, monolayer transition metal dichalcogenides, and graphene. Here, also van der Waals heterostructures (vdWh), which are stacks of different twodimensional materials, are considered. A new multi-scale approach for calculating the dielectric-function of vdWh, which extends \textit{ab initio} accuracy to the description of hundreds of atomic layers, is presented. Also, one-dimensional plasmons are studied in the case of atomically thin nanowires and edge-states of MoS$_2$.

General information

State: Published
Organisations: Department of Physics, Theoretical Atomic-scale Physics, Center for Nanostructured Graphene
Authors: Winther, K. T. (Intern), Thygesen, K. S. (Intern), Jacobsen, K. W. (Intern)
Number of pages: 156
Publication date: 2015

Publication information

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Publication: Research › Ph.D. thesis – Annual report year: 2015

Quiet swimming at low Reynolds number

The stresslet provides a simple model of the flow created by a small, freely swimming and neutrally buoyant aquatic organism and shows that the far field fluid disturbance created by such an organism in general decays as one over distance squared. Here we discuss a quieter swimming mode that eliminates the stresslet component of the flow and leads to a faster spatial decay of the fluid disturbance described by a force quadrupole that decays as one over distance cubed. Motivated by recent experimental results on fluid disturbances due to small aquatic organisms, we demonstrate that a three-Stokeslet model of a swimming organism which uses breast stroke type kinematics is an example of such a quiet swimmer. We show that the fluid disturbance in both the near field and the far field is significantly reduced by appropriately arranging the propulsion apparatus, and we find that the far field power laws are valid surprisingly close to the organism. Finally, we discuss point force models as a general framework for hypothesis generation and experimental exploration of fluid mediated predator-prey interactions in the planktonic world.

General information

State: Published
Organisations: Department of Physics, Biophysics and Fluids, Centre for Ocean Life, National Institute of Aquatic Resources
Authors: Andersen, A. P. (Intern), Wadhwa, N. (Intern), Kiørboe, T. (Intern)
Number of pages: 5
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information

Journal: Physical Review E
Volume: 91
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ISSN (Print): 2470-0045
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BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
Recent Academic Heritage at Universities

General information
State: Published
Organisations: Department of Physics
Authors: Zwisler, L. (Intern)
Publication date: 2015
Recent ASDEX Upgrade research in support of ITER and DEMO

Recent experiments on the ASDEX Upgrade tokamak aim at improving the physics base for ITER and DEMO to aid the machine design and prepare efficient operation. Type I edge localized mode (ELM) mitigation using resonant magnetic perturbations (RMPs) has been shown at low pedestal collisionality. In contrast to the previous high $v^*$ regime, suppression only occurs in a narrow RMP spectral window, indicating a resonant process, and a concomitant confinement drop is observed due to a reduction of pedestal top density and electron temperature. Strong evidence is found for the ion heat flux to be the decisive element for the L–H power threshold. A physics based scaling of the density at which the minimum PLH occurs indicates that ITER could take advantage of it to initiate H-mode at lower density than that of the final Q = 10 operational point. Strong evidence is found for the ion heat flux to be the decisive element for the L–H power threshold. A physics based scaling of the density at which the minimum PLH occurs indicates that ITER could take advantage of it to initiate H-mode at lower density than that of the final Q = 10 operational point. Core density fluctuation measurements resolved in radius and wave number show that an increase of $\rho/L_{Te}$ introduced by off-axis electron cyclotron resonance heating (ECRH) mainly increases the large scale fluctuations. The radial variation of the fluctuation level is in agreement with simulations using the GENE code. Fast particles are shown to undergo classical slowing down in the absence of large scale magnetohydrodynamic (MHD) events and for low heating power, but show signs of anomalous radial redistribution at large heating power, consistent with a broadened off-axis neutral beam current drive current profile under these conditions. Neoclassical tearing mode (NTM) suppression experiments using electron cyclotron current drive (ECCD) with feedback controlled deposition have allowed to test several control strategies for ITER, including automated control of (3,2) and (2,1) NTMs during a single discharge. Disruption mitigation studies using massive gas injection (MGI) can show an increased fuelling efficiency with high field side injection, but a saturation of the fuelling efficiency is observed at high injected mass as needed for runaway electron suppression. Large locked modes can significantly decrease the fuelling efficiency and increase the asymmetry of radiated power during MGI mitigation. Concerning power exhaust, the partially detached ITER divertor scenario has been demonstrated at $P_{\text{sep}}/R = 10$ MW m$^{-1}$ in ASDEX Upgrade, with a peak time averaged target load around 5 MW m$^{-2}$, well consistent with the component limits for ITER. Developing this towards DEMO, full detachment was achieved at $P_{\text{sep}}/R = 7$ MW m$^{-1}$ and stationary discharges with core radiation fraction of the order of DEMO requirements (70% instead of the 30% needed for ITER) were demonstrated. Finally, it remains difficult to establish the standard ITER Q = 10 scenario at low $q_{95} = 3$ in the all-tungsten (all-W) ASDEX Upgrade due to the observed poor confinement at low $\beta_N$. This is mainly due to a degraded pedestal performance and hence investigations at shifting the operational point to higher $\beta_N$ by lowering the current have been started. At higher $q_{95}$, pedestal performance can be recovered by seeding N$_2$ as well as CD$_4$, which is interpreted as improved pedestal stability due to the decrease of bootstrap current with increasing Zeff. Concerning advanced scenarios, the upgrade of ECRH power has allowed experiments with central ctr-ECCD to modify the q-profile in improved H-mode scenarios, showing an increase in confinement at still good MHD stability with flat elevated q-profiles at values between 1.5 and 2.
Recent Development in Hydrogen Evolution Reaction Catalysts and Their Practical Implementation

The past 10 years have seen great advances in the field of electrochemical hydrogen evolution. In particular, several new nonprecious metal electrocatalysts, for example, the MoS2 or the Ni2P family of materials, have emerged as contenders for electrochemical hydrogen evolution under harsh acidic conditions offering nearly platinum like catalytic performance. The developments have been particularly fast in the last 5 years, and the present Perspective highlights key developments and discusses them, along with hydrogen evolution in general, in the context of the global energy problem.

General information

State: Published
Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics, Center for Individual Nanoparticle Functionality
Authors: Vesborg, P. C. K. (Intern), Seger, B. (Intern), Chorkendorff, I. (Intern)
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Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 8.18 SJR 4.602 SNIP 1.651
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 4.143 SNIP 1.758 CiteScore 8.04
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Reduction of a Ni/Spinel Catalyst for Methane Reforming

A nickel/spinel (Ni/MgAl2O4) catalyst, w(Ni) = 22 wt%, was investigated in situ during reduction with wide angle X-ray scattering (WAXS) in a laboratory setup and with anomalous small angle X-ray scattering (ASAXS) at a synchrotron source. Complementary high resolution transmission electron microscopy (HRTEM) was performed on the fresh catalyst sample. The Ni particles in the fresh catalyst sample were observed to exhibit a Ni/ NiO core/shell structure. A decrease of the Ni lattice parameter is observed during the reduction in a temperature interval from 413 – 453 K, which can be related to the reduction of the NiO shell, whereby stress due to the lattice mismatch of Ni and NiO is relieved.
Reduction of thermal budget in the solar industry
Relating Direct Methanol Fuel Cell Performance to Measurements in a Liquid Half Cell

Direct methanol fuel cells (DMFC) could act as a replacement for batteries in low power electronics. For instance, micro—DMFC’s could be used to power hearing instruments[1]. The power output of a DMFC is limited by the sluggish kinetics of both the methanol oxidation reaction (MOR) on the anode and the oxygen reduction reaction (ORR) on the cathode. Thus far, to achieve high power densities with a single cell, the catalyst loadings have been increased much as possible (20 mg/cm² PtRu/C on anode and 4 mg/cm² Pt/C on cathode). More active catalysts would yield higher power densities which in turn would allow further miniaturization or powering more advanced and more power hungry devices. The activity of fuel cell catalysts is often probed in the form of thin films in liquid half cells. However, it is challenging to mimic the conditions in an actual DMFC. On the other hand, it can also be problematic to extract the catalyst activity from a fuel cell measurement. In this work, we attempt to narrow the gap between fuel cell testing and liquid half-cell measurements. First, by placing a custom reference electrode within the fuel cell, we can determine the potential at the anode and cathode under in-operando conditions. This in turn, allows us to directly correlate our measurements to those performed in a liquid half-cell at the same potential. For our half-cell measurements, we have tested different catalysts (Pt/C, PtRu/C) for the methanol oxidation reaction (MOR) and the oxygen reduction reaction (ORR) in the presence of methanol. By comparing the two measurements, we make recommendations for performing liquid half-cell measurements under realistic conditions. [1] J.H. Hales, C. Kalleøe, T. Lund-Olesen, A.-C. Johansson, H.C. Fanøe, Y. Yu, et al., Micro fuel cells power the hearing aids of the future, Fuel Cells Bull. 2012 (2012) 12–16. doi:10.1016/S1464-2859(12)70367-X.

Removal of low concentration contaminant species using photocatalysis: Elimination of ethene to sub-ppm levels with and without water vapor present

A photocatalytic model reactor system has been devised to assess the capacity and feasibility of a photocatalytic unit for the removal of trace amounts of organic contaminants in air. Realistic operating conditions are applied, and a mathematical model based on Langmuir–Hinselwood adsorption permits the capacity of the removal unit to be extrapolated to extreme operating conditions. A radial flow reactor system allows parameters such as gas velocity,
contaminant concentration and relative humidity to be accurately controlled. Ethene photooxidation in fruit containers is studied as an example of application. A runaway ethene production from a full shipment of fruit in a 40’ container can be prevented from a starting ethene concentration of 0.5 ppm with a few m\(^2\) of the porous photocatalyst at a 254 nm irradiance of 37.5 mWcm\(^{-2}\).

**General information**

*State:* Published
*Organisations:* Department of Physics, Experimental Surface and Nanomaterials Physics, Department of Micro- and Nanotechnology, Silicon Microtechnology
*Authors:* Nielsen, M. G. (Intern), Vesborg, P. C. K. (Intern), Hansen, O. (Intern), Chorkendorff, I. (Intern)
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  - Web of Science (2018): Indexed yes
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  - Web of Science (2016): Indexed yes
  - BFI (2015): BFI-level 2
  - Scopus rating (2015): CiteScore 5.68
  - Web of Science (2015): Indexed yes
  - BFI (2014): BFI-level 2
  - Scopus rating (2014): CiteScore 4.92
  - Web of Science (2014): Indexed yes
  - BFI (2013): BFI-level 1
  - Scopus rating (2013): CiteScore 4.59
  - ISI indexed (2013): ISI indexed yes
  - Web of Science (2013): Indexed yes
  - BFI (2012): BFI-level 1
  - Scopus rating (2012): CiteScore 3.92
  - ISI indexed (2012): ISI indexed yes
  - Web of Science (2012): Indexed yes
  - BFI (2011): BFI-level 1
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  - ISI indexed (2011): ISI indexed yes
  - Web of Science (2011): Indexed yes
  - BFI (2010): BFI-level 1
  - Web of Science (2010): Indexed yes
  - BFI (2009): BFI-level 1
  - Web of Science (2009): Indexed yes
  - BFI (2008): BFI-level 2
  - Web of Science (2008): Indexed yes
  - Web of Science (2007): Indexed yes
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  - Web of Science (2003): Indexed yes
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Reply to 'Discrete and continuous variables for measurement-device-independent quantum cryptography'

General information
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Organisations: Department of Physics, Quantum Physics and Information Technology, University of York, University of Toronto, Massachusetts Institute of Technology
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Main Research Area: Technical/natural sciences

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Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 21.32 SJR 15.689 SNIP 9.187
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 14.588 SNIP 9.701 CiteScore 17.25
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 13.474 SNIP 7.954 CiteScore 13.46
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 10.7 SNIP 8.239
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 8.746 SNIP 11.493
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 6.83 SNIP 7.606
Reversible Guest Binding in a Non-Porous Fe\textsuperscript{II} Coordination Polymer Host Toggles Spin Crossover

Formation of either a dimetallic compound or a 1\,D coordination polymer of adiponitrile adducts of [Fe(bpte)]\textsuperscript{2+} (bpte=[1,2-bis(pyridin-2-ylmethyl)thio]ethane) can be controlled by the choice of counteranion. The iron(II) atoms of the bis(adiponitrile)-bridged dimeric complex [Fe\textsubscript{2}(bpte)\textsubscript{2}(\mu\textsubscript{2}-NC(CH\textsubscript{2})\textsubscript{4}CN)\textsubscript{2}]\textsubscript{2}(SbF\textsubscript{6})\textsubscript{4} (2) are low spin at room temperature, as are those in the polymeric adiponitrile-linked acetone solvate polymer [(Fe(bpte)(\mu\textsubscript{2}-NC(CH\textsubscript{2})\textsubscript{4}CN)-BPh\textsubscript{4})\textsubscript{2}⋅Me\textsubscript{2}CO] (3⋅Me\textsubscript{2}CO). On heating 3⋅Me\textsubscript{2}CO to 80°C, the acetone is abruptly removed with an accompanying purple to dull lavender colour change corresponding to a conversion to a high-spin compound. Cooling reveals that the desolvate 3 shows hysteretic and abrupt spin crossover (SCO) S=0↔S=2 behaviour centred at 205 K. Non-porous 3 can reversibly absorb one equivalent of acetone per iron centre to regenerate the same crystalline phase of 3⋅Me\textsubscript{2}CO concurrently reinstating a low-spin state.

General information

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Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Chalmers University of Technology, University of Sydney, University of Copenhagen, University of Southern Denmark
Authors: Lennartson, A. (Ekstern), Southon, P. (Ekstern), Sciortino, N. F. (Ekstern), Kepert, C. J. (Ekstern), Frandsen, C. (Intern), Mørup, S. (Intern), Piligkos, S. (Ekstern), McKenzie, C. J. (Ekstern)
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): SNIP 1.02 SJR 2.265 CiteScore 4.9
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 5.03 SJR 2.352 SNIP 1.068
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 2.461 SNIP 1.195 CiteScore 4.99
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.526 SNIP 1.222 CiteScore 5.51
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.643 SNIP 1.239 CiteScore 5.68
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 2.935 SNIP 1.291 CiteScore 5.55
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
Role of Li$_2$O$_2$@Li$_2$CO$_3$ Interfaces on Charge Transport in Nonaqueous Li–Air Batteries

The formation and oxidation of the main discharge product in nonaqueous secondary Li–O$_2$ batteries, that is, Li$_2$O$_2$, has been studied intensively, but less attention has been given to the formation of cathode–electrolyte interfaces, which can significantly influence the performance of the Li–O$_2$ battery. Here we apply density functional theory with the Hubbard U correction (DFT+U) and nonequilibrium Green's function (NEGF) methods to investigate the role of Li$_2$O$_2$@Li$_2$CO$_3$ interface layers on the ionic and electronic transport properties at the oxygen electrode. We show that, for example, lithium vacancies accumulate at the peroxide part of the interface during charge, reducing the coherent electron transport by two to three orders of magnitude compared with pristine Li$_2$O$_2$. During discharge, Li$_2$O$_2$@Li$_2$CO$_3$ interfaces may, however, provide an alternative in-plane channel for fast electron polaron hopping that could improve the electronic conductivity and ultimately increase the practical capacity in nonaqueous Li–O$_2$ batteries.
Sacrificial structures for deep reactive ion etching of high-aspect ratio kinoform silicon x-ray lenses

This article describes the realization of complex high-aspect ratio silicon structures with feature dimensions from 100 μm to 100 nm by deep reactive ion etching using the Bosch process. As the exact shape of the sidewall profiles can be crucial for the proper functioning of a device, the authors investigated how sacrificial structures in the form of guarding walls and pillars may be utilized to facilitate accurate control of the etch profile. Unlike other sacrificial structuring approaches, no silicon-on-insulator substrates or multiple lithography steps are required. In addition, the safe removal of the sacrificial structures was accomplished by thermal oxidation and subsequent selective wet etching. The effects of the dimensions and relative placement of sacrificial walls and pillars on the etching result were determined through systematic experiments. The authors applied this process for exact sidewall control in the manufacture of x-ray lenses that are very sensitive to sidewall shape nonuniformities. Compound kinoform lenses for focusing hard x-rays with structure heights of 200 μm were manufactured, and the lenses were tested in terms of their focusing ability and refracting qualities using synchrotron radiation at a photon energy of 17 keV. A 180 μm long line focus with a waist of 430 nm at a focal length of 215 mm was obtained.

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Scopus rating (2017): SNIP 0.631 SJR 0.467 CiteScore 1.25
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.08 SJR 0.595 SNIP 0.691
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.533 SNIP 0.641 CiteScore 0.66
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.509 SNIP 0.601 CiteScore 0.61
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.55 SNIP 0.631 CiteScore 0.83
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.691 SNIP 0.717 CiteScore 0.85
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.868 SNIP 0.857 CiteScore 1.22
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.9 SNIP 0.852
Web of Science (2010): Indexed yes
Scalability and feasibility of photoelectrochemical \( \text{H}_2 \) evolution: the ultimate limit of Pt nanoparticle as an HER catalyst
The recent surge in investigating electrocatalysts for the \( \text{H}_2 \) evolution reaction is based on finding a cheap alternative to Pt. However platinum’s excellent catalytic activity means very little catalyst needs to be used. The present study combines model experiments with numerical modeling to determine exactly how little catalyst is needed. Specifically we investigate ultra-low Pt loadings for use in photoelectrochemical \( \text{H}_2 \) evolution using \( \text{TiO}_2-\text{Ti-pn}\) Si photocathodes. At a current density of 10 mA cm\(^{-2}\), we photocathodically evolve \( \text{H}_2 \) at +465, +450, +350 and +270 mV vs., RHE at Pt loadings of 1000, 200, 50, and 10 ng cm\(^{-2}\) corresponding to HER overpotentials of \( \eta_{1000\text{ng}} = 32 \) mV, \( \eta_{200\text{ng}} = 46 \) mV, \( \eta_{50\text{ng}} = 142 \) mV, and \( \eta_{10\text{ng}} = 231 \) mV. To put this in perspective, if 30% of the world’s current annual Pt production was used for \( \text{H}_2 \) evolution catalysis, using a loading of 100 ng cm\(^{-2}\) and a current of 10 mA cm\(^{-2}\) would produce 1 TW\(_{\text{average}}\) of \( \text{H}_2 \). The photoelectrochemical data matched the modeling calculations implying that we were near the fundamental maximum in performance for our system. Furthermore modeling indicated that the overpotentials were dominated by mass transfer effects, rather than catalysis unless catalyst loadings were less than 1000 ng cm\(^{-2}\).

General information
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Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics, Department of Micro- and Nanotechnology, Silicon Microtechnology, Aalto University
Authors: Kemppainen, E. (Ekstern), Bodin, A. (Intern), Sebök, B. (Intern), Pedersen, T. (Intern), Seger, B. (Intern), Mei, B. T. (Intern), Bae, D. (Intern), Vesborg, P. C. K. (Intern), Halme, J. (Ekstern), Hansen, O. (Intern), Lund, P. D. (Ekstern), Chorkendorff, I. (Intern)
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Scaling of phloem structure and optimality of photoassimilate transport in conifer needles

The phloem vascular system facilitates transport of energy-rich sugar and signalling molecules in plants, thus permitting long-range communication within the organism and growth of non-photosynthesizing organs such as roots and fruits. The flow is driven by osmotic pressure, generated by differences in sugar concentration between distal parts of the plant. The phloem is an intricate distribution system, and many questions about its regulation and structural diversity remain unanswered. Here, we investigate the phloem structure in the simplest possible geometry: a linear leaf, found, for example, in the needles of conifer trees. We measure the phloem structure in four tree species representing a diverse set of habitats and needle sizes, from 1 (Picea omorika) to 35 cm (Pinus palustris). We show that the phloem shares common traits across these four species and find that the size of its conductive elements obeys a power law. We present a minimal model that accounts for these common traits and takes into account the transport strategy and natural constraints. This minimal model predicts a power law phloem distribution consistent with transport energy minimization, suggesting that energetics are more important than translocation speed at the leaf level.
In this work we present a search for (solar) chameleons with the CERN Axion Solar Telescope (CAST). This novel experimental technique, in the field of dark energy research, exploits both the chameleon coupling to matter (βm) and to photons (βΥ) via the Primako effect. By reducing the X-ray detection energy threshold used for axions from 1 keV to 400 eV CAST became sensitive to the converted solar chameleon spectrum which peaks around 600 eV. Even though we have not observed any excess above background, we can provide a 95% C.L. limit for the coupling strength of chameleons to photons of βΥ≤10^{11} for 1 < βm < 10^{6}.
Selective CO Methanation on Ru/TiO₂ Catalysts: Role and Influence of Metal-Support Interactions

Aiming at a detailed understanding of the role of metal-support interactions in the selective methanation of CO in CO₂-rich reformate gases, we have investigated the catalytic performance of a set of Ru/TiO₂ catalysts with comparable Ru loading, Ru particle size, and TiO₂ phase composition but very different surface areas (ranging from 20 to 235 m² g⁻¹) in this reaction. The activity for CO methanation, under steady-state conditions, was found to strongly depend on the TiO₂ support surface area, increasing first with increasing surface area up to a maximum activity for the Ru/TiO₂ catalyst with a surface area of 121 m² g⁻¹ and then decreasing for an even higher surface area; however, the selectivity is mainly determined by the Ru particle size, which slightly decreases with increasing support surface area. This goes along with an increase in selectivity for CO methanation, in agreement with a model proposed previously for nonreducible supports. In situ infrared measurements further revealed that also the adsorption properties for these catalysts, as evidenced by the CO adsorption strength, change significantly with increasing catalyst surface area and that strong metal-support interactions cause a partial overgrowth of the Ru nanoparticles for the highest surface area catalyst. The interplay between catalyst surface area and reaction characteristics and the important role of metal-support interactions in the reaction, in addition to particle size effects, will be elucidated and discussed.
Self-organized criticality revisited: non-local transport by turbulent amplification

We revise the applications of self-organized criticality (SOC) as a paradigmatic model for tokamak plasma turbulence. The work, presented here, is built around the idea that some systems do not develop a pure critical state associable with SOC, since their dynamical evolution involves as a competing key factor an inverse cascade of the energy in reciprocal space. Then relaxation of slowly increasing stresses will give rise to intermittent bursts of transport in real space and outstanding transport events beyond the range of applicability of the 'conventional' SOC. Also, we are concerned with the causes and origins of non-local transport in magnetized plasma, and show that this type of transport occurs naturally in self-consistent strong turbulence via a complexity coupling to the inverse cascade. We expect these coupling phenomena to occur in the parameter range of strong nonlinearity and time scale separation when the Rhines time in the system is small compared with the instability growth time.

General information
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Organisations: Department of Physics, Plasma Physics and Fusion Energy, Russian Academy of Sciences
Authors: Milovanov, A. V. (Ekstern), Rasmussen, J. J. (Intern)
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Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 0.74 SJR 0.453 SNIP 0.721
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.318 SNIP 0.612 CiteScore 0.76
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.334 SNIP 0.549 CiteScore 0.77
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.304 SNIP 0.536 CiteScore 0.75
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.403 SNIP 0.532 CiteScore 0.75
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.51 SNIP 0.733 CiteScore 0.83
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.382 SNIP 0.466
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.44 SNIP 0.439
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.441 SNIP 0.496
Scopus rating (2007): SJR 0.541 SNIP 0.647
Scopus rating (2006): SJR 0.427 SNIP 0.557
Scopus rating (2005): SJR 0.443 SNIP 0.805
Scopus rating (2004): SJR 0.487 SNIP 0.748
Scopus rating (2003): SJR 0.632 SNIP 0.811
Scopus rating (2002): SJR 0.369 SNIP 0.413
Scopus rating (2001): SJR 0.473 SNIP 0.478
Scopus rating (2000): SJR 0.435 SNIP 0.759
Scopus rating (1999): SJR 0.443 SNIP 0.592

SERS sensing of plant materials

General information
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Organisations: Department of Physics, Department of Micro- and Nanotechnology, Fluidic Array Systems and Technology
Authors: Espina Palanco, M. (Intern), Mogensen, K. B. (Intern), Kneipp, K. (Intern)
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Publication date: 2015
Event: Abstract from 2nd Optical Nanospectroscopy Conference, Dublin, Ireland.
Main Research Area: Technical/natural sciences
Electronic versions:
Abstract_Marta_espina.pdf

Relations
Activities:
2nd Optical Nanospectroscopy Conference
Publication: Research › Conference abstract for conference – Annual report year: 2015
Shape-Selection of Thermodynamically Stabilized Colloidal Pd and Pt Nanoparticles Controlled via Support Effects

Colloidal chemistry, in combination with nanoparticle (NP)/support epitaxial interactions is used here to synthesize shape-selected and thermodynamically stable metallic NPs over a broad range of NP sizes. The morphology of three-dimensional palladium and platinum NPs supported on TiO2(110) was investigated using scanning tunneling microscopy. Well-defined Pd and Pt NPs were synthesized via inverse micelle encapsulation. The initially spherical NPs were found to become faceted and form an epitaxial relationship with the support after high-temperature annealing (e.g., 1100 degrees C). Shape selection was achieved for almost all Pd NPs, namely, a truncated octahedron shape with (111) top and interfacial facets. The Pt NPs were however found to adopt a variety of shapes. The epitaxial relationship of the NPs with the support was evidenced by the alignment of the cluster's edges with TiO2(110)-[001] atomic rows and was found to be responsible for the shape control. The ability of synthesizing thermally stable shape-selected metal NPs demonstrated here is expected to be of relevance for applications in the field of catalysis, since the activity and selectivity of NP catalysts has been shown to strongly depend on the NP shape.
Sharp-interface model of electrodeposition and ramified growth

We present a sharp-interface model of two-dimensional ramified growth during quasisteady electrodeposition. Our model differs from previous modeling methods in that it includes the important effects of extended space-charge regions and nonlinear electrode reactions. The electrokinetics is described by a continuum model, but the discrete nature of the ions is taken into account by adding a random noise term to the electrode current. The model is validated by comparing its behavior in the initial stage with the predictions of a linear stability analysis. The main limitations of the model are the restriction to two dimensions and the assumption of quasisteady transport.

General information
State: Published
Organisations: Department of Physics, Biophysics and Fluids
Authors: Nielsen, C. P. (Intern), Bruus, H. (Intern)
Number of pages: 15
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BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 0.987 SJR 0.979 CiteScore 2.14
Web of Science (2017): Indexed Yes
Scopus rating (2016): CiteScore 1.95 SJR 1.271 SNIP 1.018
Web of Science (2016): Indexed yes
Scopus rating (2015): SJR 1.183 SNIP 1.043 CiteScore 1.89
Web of Science (2015): Indexed yes
Scopus rating (2014): SJR 1.244 SNIP 1.135 CiteScore 2.05
Web of Science (2014): Indexed yes
Scopus rating (2013): SJR 1.307 SNIP 1.214 CiteScore 2.28
ISI indexed (2013): ISI indexed yes
Simulation of transition dynamics to high confinement in fusion plasmas

The transition dynamics from the low (L) to the high (H) confinement mode in magnetically confined plasmas is investigated using a first-principles four-field fluid model. Numerical results are in agreement with measurements from the Experimental Advanced Superconducting Tokamak - EAST. Particularly, the slow transition with an intermediate dithering phase is well reproduced at proper parameters. The model recovers the power threshold for the L-H transition as well as the decrease in power threshold switching from single to double null configuration observed experimentally. The results are highly relevant for developing predictive models of the transition, essential for understanding and optimizing future fusion power reactors.
Simulation of waviness in neutron guides

As the trend of neutron guide designs points towards longer and more complex guides, imperfections such as waviness becomes increasingly important. Simulations of guide waviness has so far been limited by a lack of reasonable waviness models. We here present a stochastic description of waviness and its implementation in the McStas simulation package. The effect of this new implementation is compared to the guide simulations without waviness and the simple, yet unphysical, waviness model implemented in McStas 1.12c and 2.0.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, University of Copenhagen
Authors: Hansen, U. B. (Ekstern), Bertelsen, M. (Ekstern), Bergbäck Knudsen, E. (Intern), Lefmann, K. (Ekstern)
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Journal: Journal of Neutron Research
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BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 0.425 SJR 0.283 CiteScore 0.53
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 0.85 SJR 0.286 SNIP 1.219
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.286 SNIP 1.92 CiteScore 0.88
BFI (2014): BFI-level 1
Web of Science (2014): Indexed yes
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ISI indexed (2013): ISI indexed no
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ISI indexed (2012): ISI indexed no
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.327 SNIP 2.092
ISI indexed (2011): ISI indexed no
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.18 SNIP 0.274
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.177 SNIP 0.545
BFI (2008): BFI-level 1
Simulations of super-structure domain walls in two dimensional assemblies of magnetic nanoparticles

We simulate the formation of domain walls in two-dimensional assemblies of magnetic nanoparticles. Particle parameters are chosen to match recent electron holography and Lorentz microscopy studies of almost monodisperse cobalt nanoparticles assembled into regular, elongated lattices. As the particles are small enough to consist of a single magnetic domain each, their magnetic interactions can be described by a spin model in which each particle is assigned a macroscopic "superspin." Thus, the magnetic behaviour of these lattices may be compared to magnetic crystals with nanoparticle superspins taking the role of the atomic spins. The coupling is, however, different. The superspins interact only by dipolar interactions as exchange coupling between individual nanoparticles may be neglected due to interparticle spacing. We observe that it is energetically favorable to introduce domain walls oriented along the long dimension of nanoparticle assemblies rather than along the short dimension. This is unlike what is typically observed in continuous magnetic materials, where the exchange interaction introduces an energetic cost proportional to the area of the domain walls. Structural disorder, which will always be present in realistic assemblies, pins longitudinal domain walls when the external field is reversed, and makes a gradual reversal of the magnetization by migration of longitudinal domain walls possible, in agreement with previous experimental results.

General information
State: Published
Organisations: Department of Physics, Center for Electron Nanoscopy, Experimental Surface and Nanomaterials Physics, Neutrons and X-rays for Materials Physics
Authors: Jordanovic, J. (Intern), Beleggia, M. (Intern), Schiøtz, J. (Intern), Frandsen, C. (Intern)
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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
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.484 SNIP 1.204
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.51 SNIP 1.237
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.644 SNIP 1.326
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.695 SNIP 1.387
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.944 SNIP 1.667
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 2.055 SNIP 1.605
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 2.128 SNIP 1.591
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 2.078 SNIP 1.532
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
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Single-Molecule Electrochemical Transistor Utilizing a Nickel-Pyridyl Spinterface

Using a scanning tunnelling microscope break-junction technique, we produce 4,4′-bipyridine (44BP) single-molecule junctions with Ni and Au contacts. Electrochemical control is used to prevent Ni oxidation and to modulate the conductance of the devices via non-redox gating - the first time this has been shown using non-Au contacts. Remarkably the conductance and gain of the resulting Ni-44BP-Ni electrochemical transistors is significantly higher than analogous Au-based devices. Ab-initio calculations reveal that this behavior arises because charge transport is mediated by spin-polarized Ni d-electrons, which hybridize strongly with molecular orbitals to form a "spinterface". Our results highlight the important role of the contact material for single-molecule devices and show that it can be varied to provide control of charge and spin transport.
Life in the ocean is shaped by the trade-off between a need to encounter other organisms for feeding or mating, and to avoid encounters with predators. Avoiding or achieving encounters necessitates an efficient means of collecting the maximum possible information from the surroundings through the use of remote sensing. In this study, we explore how sensing mode and range depend on body size. We reveal a hierarchy of sensing modes (chemosensing, mechanosensing, vision, hearing, and echolocation) where body size determines the available battery of sensing modes and where larger body size means a longer sensing range. The size-dependent hierarchy and the transitions between primary sensory modes are explained on the grounds of limiting factors set by physiology and the physical laws governing signal generation, transmission and reception. We characterize the governing mechanisms and theoretically predict the body size limits for various sensory modes, which align very well with size ranges found in literature. The treatise of all ocean life, from unicellular organisms to whales, demonstrates how body size determines available sensing modes, and thereby acts as a major structuring factor of aquatic life.
Slower phloem transport in gymnosperm trees can be attributed to higher sieve element resistance

In trees, carbohydrates produced in photosynthesizing leaves are transported to roots and other sink organs over distances of up to 100 m inside a specialized transport tissue, the phloem. Angiosperm and gymnosperm trees have a fundamentally different phloem anatomy with respect to cell size, shape and connectivity. Whether these differences have an effect on the physiology of carbohydrate transport, however, is not clear. A meta-analysis of the experimental data on phloem transport speed in trees yielded average speeds of 56 cm h⁻¹ for angiosperm trees and 22 cm h⁻¹ for gymnosperm trees. Similar values resulted from theoretical modeling using a simple transport resistance model. Analysis of the model parameters clearly identified sieve element (SE) anatomy as the main factor for the significantly slower carbohydrate transport speed inside the phloem in gymnosperm compared with angiosperm trees. In order to investigate the influence of SE anatomy on the hydraulic resistance, anatomical data on SEs and sieve pores were collected by transmission electron microscopy analysis and from the literature for 18 tree species. Calculations showed that the hydraulic resistance is significantly higher in the gymnosperm than in angiosperm trees. The higher resistance is only partially offset by the considerably longer SEs of gymnosperms.
Solar Fuels: A quick look at how photoelectrodes work.

General information
State: Published
Organisations: Department of Micro- and Nanotechnology, Department of Physics, Experimental Surface and Nanomaterials Physics
Authors: Hansen, O. (Intern), Seger, B. (Intern), Vesborg, P. C. K. (Intern), Chorkendorff, I. (Intern)
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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
Solid solution barium–strontium chlorides with tunable ammonia desorption properties and superior storage capacity

Metal halide ammines are very attractive materials for ammonia absorption and storage—applications where the practically accessible or usable gravimetric and volumetric storage densities are of critical importance. Here we present, that by combining advanced computational materials prediction with spray drying and in situ thermogravimetric and structural characterization, we synthesize a range of new, stable barium-strontium chloride solid solutions with superior ammonia storage densities. By tuning the barium/strontium ratio, different crystallographic phases and compositions can be obtained with different ammonia ab- and desorption properties. In particular it is shown, that in the molar range of 35–50% barium and 65–50% strontium, stable materials can be produced with a practically usable ammonia density (both volumetric and gravimetric) that is higher than any of the pure metal halides, and with a practically accessible volumetric ammonia densities in excess of 99% of liquid ammonia.

General information
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Organisations: Department of Physics, Center for Atomic-scale Materials Design, Department of Energy Conversion and Storage, Atomic scale modelling and materials, Amminex Emissions Technology A/S
Authors: Bialy, A. (Ekstern), Jensen, P. B. (Intern), Blanchard, D. (Intern), Vegge, T. (Intern), Quaade, U. J. (Ekstern)
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Scopus rating (2017): SNIP 0.805 SJR 0.632 CiteScore 2.2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.09 SJR 0.618 SNIP 0.871
Solid State Structure of Poly(9,9-dinonylfluorene)

We report on X-ray diffraction and grazing-incidence X-ray diffraction data of poly(9,9-dinonylfluorene) (PF9) in bulk, thin films and in the 1% methylcyclohexane gel. We denote the main crystalline phase as alpha phase and propose that the unit cell is monoclinic (a = 29.31 angstrom, b = 23.65 angstrom, c = 33.33 angstrom, and gamma = 84.70 degrees) in bulk and orthorhombic (a = 28.70 angstrom, b = 23.48 angstrom, and c = 33.23 angstrom) in thin films. This structure
corresponds to the layered structure along the a-axis (along the elongated side chains and perpendicular to the seemingly stiff polymer chains) and to the stacking of aromatic main chain units along the b-axis. The polymer chains are aligned along the c-axis. Monoclinic structure agrees with the layer spacing of 14.6 angstrom, the stacking period d(040) = 5.89 angstrom and the monomer repeat distance of 8.33 angstrom. The alpha phase experiences an order-disorder transition at 170 degrees C upon heating. In the 1% methylcydohexane gel, this structural motif is maintained but with the loss of long-range order. This is interpreted as a formation of mesomorphic beta phase with an orthorhombic unit cell (a = 29.1 angstrom, b = 28.1 angstrom, and c = 16.7 angstrom). Structural analogues to other 9,9-di-n-alkyl-substituted polyfluorenes are discussed in terms of unit cell parameters and backbone geometry.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, University of Helsinki, Bergische Universität Wuppertal
Authors: Torkkeli, M. (Ekstern), Galbrecht, F. (Ekstern), Scherf, U. (Ekstern), Knaapila, M. (Intern)
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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
Spin polarization versus color–flavor locking in high-density quark matter

It is shown that spin polarization with respect to each flavor in three-flavor quark matter occurs instead of color–flavor locking at high baryon density by using the Nambu–Jona-Lasinio model with four-point tensor-type interaction. Also, it is indicated that the order of phase transition between the color–flavor-locked phase and the spin-polarized phase is the first order by means of second-order perturbation theory.
Spontaneous magnetization in high-density quark matter

It is shown that spontaneous magnetization occurs due to the anomalous magnetic moments of quarks in high-density quark matter under the tensor-type four-point interaction. The spin polarized condensate for each flavor of quark appears at high baryon density, which leads to the spontaneous magnetization due to the anomalous magnetic moments of quarks. The implications for the strong magnetic field in compact stars is discussed.

General information

State: Published
Organisations: Department of Physics, Biophysics and Fluids, University of Coimbra
Authors: Tsue, Y. (Ekstern), da Providência, J. (Ekstern), Providência, C. (Ekstern), Yamamura, M. (Ekstern), Bohr, H. (Intern)
Publication date: 2015
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Web of Science (2018): Indexed yes
Scopus rating (2017): SNIP 0.731 SJR 0.853 CiteScore 1.61
Web of Science (2017): Indexed Yes
Scopus rating (2016): SJR 0.857 SNIP 0.697 CiteScore 1.02
Web of Science (2016): Indexed yes
Scopus rating (2015): SJR 1.007 SNIP 0.825 CiteScore 0.99
Web of Science (2015): Indexed yes
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Spray—coated CZTS Nanoparticles In Water for Environmentally—friendly, Inexpensive Solar Cell Absorber Material

General information
Squeezing-enhanced feedback cooling of a microresonator

Since its inception, quantum mechanics have not ceased to fascinate the scientific world, and especially the fundamental question about the famous Schrödinger's cat being alive or dead, or both, is still far from being answered. Although superposition states have been achieved with small particles, such as photons or atoms, they have not yet been observed on large and massive objects consisting of billions of atoms. With the advance of cavity optomechanics, the quantum behavior of massive mechanical oscillators is becoming accessible and a major key requirement in this direction is the ability to cool such oscillators into their quantum ground state. In the present work we investigate a cold damping scheme relying on the ultra-sensitive measurement of mechanical displacements, provided by a cavity-enhanced optomechanical interaction with quadrature squeezed states of light, to control strong dielectric gradient forces actuating the motion of a toroidal microresonator within a feedback loop. We first determine theoretically the conditions and limits to squeezing-enhanced measurement sensitivity of mechanical motion in a cavity optomechanical system, and perform experimentally a proof-of-principle on our microtoroids. Secondly we model the dielectric gradient force actuation scheme and investigate its capabilities in controlling the vibrations of a microtoroid acoustic mode.

Squeezing-enhanced measurement sensitivity in a cavity optomechanical system

We determine the theoretical limits to squeezing-enhanced measurement sensitivity of mechanical motion in a cavity optomechanical system. The motion of a mechanical resonator is transduced onto quadrature fluctuations of a cavity optical field and a measurement is performed on the optical field exiting the cavity. We compare measurement sensitivities obtained with coherent probing and quantum-enhanced probing of the mechanical motion, i.e. the coherent probe field carries vacuum states and quadrature squeezed vacuum states at sideband frequencies, respectively. We find that quantum-enhanced probing provides little to no improvement in motion sensing for resonators in the unresolved sideband regime but may significantly increase measurement sensitivities for resonators in the resolved sideband regime.
Star formation suppression in compact group galaxies: a new path to quenching?

We present CO(1-0) maps of 12 warm H$_2$-selected Hickson Compact Groups (HCGs), covering 14 individually imaged warm H$_2$ bright galaxies, with the Combined Array for Research in Millimeter Astronomy. We found a variety of molecular gas distributions within the HCGs, including regularly rotating disks, bars, rings, tidal tails, and possibly nuclear outflows,
though the molecular gas morphologies are more consistent with spirals and earlytype galaxies than mergers and interacting systems. Our CO-imaged HCG galaxies, when plotted on the Kennicutt-Schmidt relation, shows star formation (SF) suppression of <S> = 10 +/- 5, distributed bimodally, with five objects exhibiting suppressions of S greater than or similar to 10 and depletion timescales greater than or similar to 10 Gyr. This SF inefficiency is also seen in the efficiency per freefall time of Krumholz et al. We investigate the gas-to-dust ratios of these galaxies to determine if an incorrect L_CO - M(H2) conversion caused the apparent suppression and find that HCGs have normal gas-to-dust ratios. It is likely that the cause of the apparent suppression in these objects is associated with shocks injecting turbulence into the molecular gas, supported by the fact that the required turbulent injection luminosity is consistent with the bright H2 luminosity reported by Cluver et al. Galaxies with high SF suppression (S greater than or similar to 10) also appear to be those in the most advanced stages of transition across both optical and infrared color space. This supports the idea that at least some galaxies in HCGs are transitioning objects, where a disruption of the existing molecular gas in the system suppresses SF by inhibiting the molecular gas from collapsing and forming stars efficiently. These observations, combined with recent work on poststarburst galaxies with molecular reservoirs, indicates that galaxies do not need to expel their molecular reservoirs prior to quenching SF and transitioning from blue spirals to red early-type galaxies. This may imply that SF quenching can occur without the need to starve a galaxy of cold gas first.
**Stellarators and small, modular fusion power plants: New ideas for sustainable fusion power**

**General information**
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Organisations: Department of Physics, Plasma Physics and Fusion Energy, Tokamak Energy
Authors: Naulin, V. (Intern), Rasmussen, J. J. (Intern), Gryaznevich, M. (Ekstern)
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Poster presentation
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2015

**Strain sensitivity of band gaps of Sn-containing semiconductors**
Tuning of band gaps of semiconductors is a way to optimize materials for applications within photovoltaics or as photocatalysts. One way to achieve this is through applying strain to the materials. We investigate the effect of strain on a range of Sn-containing semiconductors using density functional theory and many-body perturbation theory calculations. We find that the band gaps of bulk Sn oxides with SnO$_6$ octahedra are highly sensitive to volumetric strain. By applying a small isotropic strain of 2% (-2%), a decrease (increase) of band gaps as large as 0.8 to 1.0 eV are obtained. We attribute the ultrahigh strain sensitivity to the pure Sn s-state character of the conduction-band edges. Other Sn-containing compounds may show both increasing and decreasing gaps under tensile strain and we show that the behavior can be understood by analyzing the role of the Sn s states in both the valence and the conduction bands.

**General information**
State: Published
Organisations: Center for Atomic-scale Materials Design, Department of Physics
Structure, activity, and stability of platinum alloys as catalysts for the oxygen reduction reaction

In this thesis I present our work on theoretical modelling of platinum alloys as catalysts for the Oxygen Reduction Reaction (ORR). The losses associated with the kinetics of the ORR is the main bottleneck in low-temperature fuel cells for transport applications, and more active catalysts are essential for wide-spread use of this technology. Platinum alloys have shown great promise as more active catalysts, which are still stable under reaction conditions.

We have investigated these systems on multiple scales, using either Density Functional Theory (DFT) or Effective Medium Theory (EMT), depending on the length and time scales involved.

Using DFT, we show how diffusion barriers in transition metal alloys in the L12 structure depend on the alloying energy, supporting the assumption that an intrinsically more stable alloy is also more stable towards diffusion-related degradation and dealloying due to kinetic barriers, despite the thermodynamic driving force for dissolution.

This is followed by our results on trying to decouple the strain and ligand effects for platinum skin structures, and determining whether there is any correlation between adsorption energy and surface stability in these systems. We find that there is such a correlation for some adsorbates, indicating that there exists a limit for the stability of an overlayer for a given adsorption strength.

Finally, we introduce our work on platinum alloy nanoparticles, and our attempt to isolate the features which result in the increased activity that has been seen experimentally. We show how the platinum-platinum distance at the surface is decreased for a variety of alloy phases in the core, with greater compression of the overlayer for core phases with lattice parameters which are either much smaller or much larger than pure platinum.
Study of 3-D stress development in parent and twin pairs of a hexagonal close-packed polycrystal: Part I - In-situ three-dimensional synchrotron X-ray diffraction measurement

High anisotropy in the elastic and plastic properties of hexagonal close-packed (hcp) structured metals not only results in drastic stress variation across grain boundaries, but also heterogeneous distributions within grains. Understanding the mechanism of load sharing between different grains becomes more complicated when deformation twinning plays a significant role in accommodating an externally applied load. In this paper, a comprehensive study of stress development in a coarse grained strongly textured hcp polycrystal Zircaloy-2, is given using three-dimensional X-ray diffraction (3DXRD) microscopy. In-situ uniaxial straining was carried out at seven steps up to 2.7% in the macroscopic direction that favors twin formation, while center-of-mass position, crystallographic orientation, elastic strain, stress, and relative volume of each grain were measured. This information was used to reconstruct the 3D microstructure and statistically study neighborhood effects on the load sharing. The investigated volume of the sample contained 6132 grains initially, yet as a result of twin formation, 9724 grains were measured in the same volume at the last loading step. It is shown that the most favored (highest Schmid factor) twin variant contributes the most to the twin number fraction; however, if the measured local stress within each grain is used for the calculation of Schmid factor, the contribution of other variants is relatively independent of Schmid factor.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, European Synchrotron Radiation Facility, University of Oxford, Queen's University
Authors: Abdolvand, H. (Ekstern), Majkut, M. (Intern), Oddershede, J. (Intern), Wright, J. P. (Ekstern), Daymond, M. R. (Ekstern)
Pages: 246-255
Publication date: 2015
Main Research Area: Technical/natural sciences

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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
Summary of the 19th Joint EU-US Transport Task Force Workshop: Conference Report
This conference report summarizes the contributions to, and discussions at, the 19th Joint EU-US Transport Task Force workshop, held in Culham, UK, during 8-11 September 2014. The workshop was organized under six topics: momentum transport, energetic particles, challenges in modelling transport in ITER and JT60-SA, L-H transition, impurity transport and SOL transport. This report follows the same structure.
Synchrotron Based Structural Investigations of Mass-Selected PtxGd Nanoparticles and a Gd/Pt(111) Single Crystal for Electrochemical Oxygen Reduction

The sluggish kinetics of the oxygen reduction reaction (ORR) hinders the commercialization of proton exchange membrane fuel cells (PEMFC). The ORR activity is enhanced by alloying Pt with late transition 3d metals (i.e. Fe, Co, Ni, and Cu)\textsuperscript{1}. However, these compounds tend to degrade in a fuel cell by dealloying. An alternative approach is to alloy Pt with rare-earth elements. Their highly negative alloying energy may provide them with kinetic stability against dealloying under reaction conditions. A recent publication from our group reported the high ORR activity and stability of polycrystalline Pt5Gd\textsuperscript{2}. In this work, we present the experimental results of mass-selected PtxGd nanoparticles synthesized by gas aggregation after sputtering of an alloy target in an ultrahigh vacuum (UHV)\textsuperscript{3}. PtxGd nanoparticles with nominal sizes of 3, 5, 7, and 9 nm were selected using time-of-flight mass filtering and deposited on glassy carbon (GC) disk electrodes. Rotating ring disk electrode (RRDE) measurements in 0.1 M HClO\textsubscript{4} were used to measure the activity in comparison to pure Pt\textsuperscript{4}. The ORR specific activity increases with the nanoparticle size; a maximum mass activity is achieved with the 7 nm sample, ~3.6 A/mg Pt at 0.9 V. X-ray absorption spectroscopy measurements suggest that the high ORR activity is due to a compressive strain exerted by the alloy core onto the Pt overlayer at the surface. The structure formed on these types of alloys\textsuperscript{2} is further elucidated using a Gd/Pt(111) single crystal. The alloy was prepared in UHV by depositing 150 Å of Gd followed by annealing, thus simulating a bulk single crystal. It was characterized in vacuo using low energy electron diffraction, ion scattering spectroscopy, X-ray photoelectron spectroscopy and temperature programmed desorption of CO. Subsequently, the crystal was transferred to an electrochemical cell, where a 1 nm thick Pt overlayer was formed; this constitutes the active phase for oxygen reduction. Using synchrotron based grazing X-ray diffraction, we determine the structure of the alloy and the Pt overlayer. The diffraction contributions from the Pt overlayer is separated from the Pt5Gd alloy, and the analysis of both diffraction patterns are presented. By investigating such well-defined structures, we gain valuable scientific insight into the relationship between their structure and functionality. On the basis of this insight, we can develop even better catalysts for oxygen electroreduction. References 1. Chen, C. et al. Highly Crystalline Multimetallic Nanoframes with Three-Dimensional Electro catalytic Surfaces. Science 343, 1339–1343 (2014). 2. Escudero-Escribano, M. et al. Pt5Gd as a Highly Active and Stable Catalyst for Oxygen Electroreduction. J. Am. Chem. Soc. 134, 16476–16479 (2012). 3. Velazquez-Palenzuela, A. et al. The enhanced activity of mass-selected PtGd nanoparticles for oxygen electroreduction. J. Catal. [in press] (2015). doi:10.1016/j.jcat.2014.12.012 4. Perez-Alonso, F. J. et al. The Effect of Size on the Oxygen Electroreduction Activity of Mass-Selected Platinum Nanoparticles. Angew. Chem. Int. Ed. 51, 4641–4643 (2012).

General information
State: Published
Organizations: Department of Physics, Experimental Surface and Nanomaterials Physics, DTU Admission Course, Center for Electron Nanoscopy, DTU Danich, Department of Chemical and Biochemical Engineering, SLAC National Accelerator Laboratory
Number of pages: 1
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Conference: The 228th ECS Meeting , Phoenix, Arizona, United States, 11/10/2015 - 11/10/2015
Main Research Area: Technical/natural sciences
Synthesis and Characterization of FeNi/γ-Al2O3 Egg-Shell Catalyst for H2 Generation by Ammonia Decomposition

General information
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Synthesis and characterization of Fe–Ni/γ-Al2O3 egg-shell catalyst for H2 generation by ammonia decomposition

The Fe–Ni alloyed nanoparticles are a promising alternative to expensive ruthenium-based catalysts for a real-scale application of hydrogen generation by ammonia decomposition. In practical applications, millimeter-sized extrudates are used as catalyst supports, where the spatial distribution of the active phase should match with the type of reaction. In this work, a novel synthesis route was developed for the preparation of a Fe–Ni/γ-Al2O3 egg-shell catalyst. Egg-shell is a preferred profile considering the highly endothermic nature of ammonia decomposition reaction. The high viscosity of glycerol, used as a solvent during impregnation, prevents the fast migration of the Fe–Ni active phase solution toward the inner-core of γ-Al2O3, giving control over the large capillary pressures. The distribution profiles were analyzed at macroscopic scale through scanning electron microscopy mapping (SEM-EDX) and optical microscopy. A three-dimensional (3-D) reconstruction of the spherical-shaped γ-Al2O3 was achieved using X-ray micro tomography and the Fe–Ni egg-shell spatial distribution was inspected throughout the entire volume of the support body. Transmission electron microscopy (TEM) specimen preparation using focused ion beam (FIB) milling allowed to acquire high resolution images of the Ni and Fe nanoparticles on γ-Al2O3, which is particularly challenging due to the crystalline nature of this support. Distinct regions of the egg-shell catalyst were analyzed through scanning TEM (STEM) and TEM. The outer-shell region showed the presence of Fe and Ni alloyed nanoparticles with a size of approximately 5nm. The egg-shell catalyst showed significant higher activity in ammonia decomposition by converting 3 times more ammonia to equilibrium conversion than either egg-white or catalyst with uniform distribution. Moreover, the egg-shell catalyst conversion only dropped 0.05% after 10h of reaction, for a space velocity of 475ml min−1g−1.
Temperature dependent polarization reversal mechanism in 0.94(Bi$_{1/2}$Na$_{1/2}$)TiO$_3$-0.06Ba(Zr$_{0.02}$Ti$_{0.98}$)O$_3$ relaxor ceramics

The temperature at which the electric field induced long-range ordered ferroelectric state undergoes transition into the short-range ordered relaxor state, $T_{F\rightarrow R}$, is commonly defined by the onset of strong dispersion of the dielectric permittivity. However, this combined macroscopic property and structural investigation of the polarization reversal process in the prototypical lead-free relaxor 0.94(Bi$_{1/2}$Na$_{1/2}$)TiO$_3$-0.06Ba(Zr$_{0.02}$Ti$_{0.98}$)O$_3$ reveals that an applied electric field can trigger depolarization and onset of relaxor-like behavior well below $T_{F\rightarrow R}$. The polarization reversal process can as such be described as a combination of (1) ferroelectric domain switching and (2) a reversible phase transition between two polar ferroelectric states mediated by a non-polar relaxor state. Furthermore, the threshold fields of the second, mediated polarization reversal mechanism depend strongly on temperature. These results are concomitant with a continuous ferroelectric to relaxor transition occurring over a broad temperature range, during which mixed behavior is observed. The nature of polarization reversal can be illustrated in electric-field-temperature (E-T) diagrams showing the electric field amplitudes associated with different polarization reversal processes. Such diagrams are useful tools for identifying the best operational temperature regimes for a given composition in actuator applications.
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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
Scopus rating (2002): SJR 4.018 SNIP 2.414
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 4.281 SNIP 2.22
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 4.178 SNIP 2.017
The dielectric genome of van der Waals heterostructures

Vertical stacking of two-dimensional (2D) crystals, such as graphene and hexagonal boron nitride, has recently lead to a new class of materials known as van der Waals heterostructures (vdWHs) with unique and highly tunable electronic properties. Abinitio calculations should in principle provide a powerful tool for modeling and guiding the design of vdWHs, but in their traditional, form such calculations are only feasible for commensurable structures with a few layers. Here we show that the dielectric properties of realistic, incommensurable vdWHs comprising hundreds of layers can be calculated with ab-initio accuracy using a multi-scale approach where the dielectric functions of the individual layers (the dielectric building blocks) are coupled simply via their long-range Coulomb interaction. We use the method to illustrate the 2D-3D dielectric transition in multi-layer MoS$_2$ crystals, the hybridization of quantum plasmons in large graphene/hBN heterostructures, and to demonstrate the intricate effect of substrate screening on the non-Rydberg exciton series in supported WS$_2$. The dielectric building blocks for a variety of 2D crystals are available in an open database together with the software for solving the coupled electrodynamic equations.
van der Waals heterostructures, 2D materials, Density functional theory, Dielectric function, Excitons, Plasmons

The enhanced activity of mass-selected PtxGd nanoparticles for oxygen electroreduction
Mass-selected platinum–gadolinium alloy nanoparticles (PtxGd NPs) are synthesized for the first time as oxygen reduction reaction (ORR) electrocatalysts using the gas aggregation technique, under ultrahigh vacuum (UHV) conditions. The morphology of the PtxGd catalysts is characterized, and their catalytic performance toward the ORR is assessed in acidic media using a half-cell configuration. The PtxGd 8-nm catalyst shows a high activity (3.6A(mgPt)−1), surpassing the highest activity reached so far with PtxY NP catalysts. In addition, the optimum PtxGd catalyst also presents high stability, as suggested by the accelerated stability tests under ORR potential cycling. Extended X-ray absorption fine structure (EXAFS) spectroscopy measurements confirm that as-prepared PtxGd NPs are compressively strained, relative to pure Pt, and that a PtxGd core/Pt-rich shell structure is adopted after partial Gd leaching. The activity correlates strongly with the compressive strain. On that basis, we propose that the ORR enhancement is due to the compressive strain within the Pt shell induced by the alloy core. The results herein confirm the suitability of PtxGd NPs as cathode nanocatalysts for proton exchange membrane fuel cells (PEMFCs).

General information
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Publication information
Journal: Journal of Catalysis
Volume: 328
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BFI (2017): BFI-level 2
The Higgs mass derived from the U(3) Lie group

The Higgs mass value is derived from a Hamiltonian on the Lie group U(3) where we relate strong and electroweak energy scales. The baryon states of nucleon and delta resonances originate in specific Bloch wave degrees of freedom coupled to a Higgs mechanism which also gives rise to the usual gauge boson masses. The derived Higgs mass is around 125 GeV. From the same Hamiltonian, we derive the relative neutron to proton mass ratio and the N and Delta mass spectra. All compare rather well with the experimental values. We predict scarce neutral flavor baryon singlets that should be visible in scattering cross-sections for negative pions on protons, in photoproduction on neutrons, in neutron diffraction dissociation experiments and in invariant mass spectra of protons and negative pions in B-decays. The fundamental predictions are based on just one length scale and the fine structure constant. More particular predictions rely also on the weak mixing angle and the up-down quark flavor mixing matrix element. With differential forms on the measure-scaled wave function, we could generate approximate parton distribution functions for the u and d valence quarks of the proton that compare well with established experimental analysis.
The IAXO Helioscope
The IAXO (International Axion Experiment) is a fourth generation helioscope with a sensitivity, in terms of detectable signal counts, at least 10^4 better than CAST phase-I, resulting in sensitivity on gay one order of magnitude better. To achieve this performance IAXO will count on a 8-coil toroidal magnet with 60 cm diameter bores and equipped with X-ray focusing optics into 0.20 cm^2 spots coupled to ultra-low background Micromegas X-ray detectors. The magnet will be on a platform that will allow solar tracking for 12 hours per day. The next short term objectives are to prepare a Technical Design Report and to construct the first prototypes of the hardware main ingredients: demonstration coil, X-ray optics and low background detector while refining the physics case and studying the feasibility studies for Dark Matter axions.

General information
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Organisations: National Space Institute, Astrophysics, Neutrons and X-rays for Materials Physics, CEA Saclay, University of South Carolina, CERN, University of Trieste, University of Zaragoza, Lawrence Livermore National Laboratory
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Volume: 650
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ISSN (Print): 1742-6596
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BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 0.48 SJR 0.241 SNIP 0.447
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 0.45 SJR 0.24 SNIP 0.401
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.252 SNIP 0.374 CiteScore 0.35
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.264 SNIP 0.352 CiteScore 0.32
The importance of being together

General information
State: Published
Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics, Massachusetts Institute of Technology
Authors: Stephens, I. (Intern), Elias, J. S. (Ekstern), Shao-Horn, Y. (Ekstern)
Number of pages: 2
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Publication date: 2015
Main Research Area: Technical/natural sciences

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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
The influence of hot neutrals in simulations of gas puff modulation

General information
State: Published
Organisations: Department of Physics, Plasma Physics and Fusion Energy, Technical University of Denmark, Culham Science Centre
Authors: Christensen, A. (Ekstern), Madsen, J. (Intern), Naulin, V. (Intern), Rasmussen, J. J. (Intern), Salmi, A. (Ekstern), Tophøj, L. E. H. (Intern)
Number of pages: 4
Publication date: 2015

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Main Research Area: Technical/natural sciences
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The microscopic structure of charge density waves in underdoped YBa$_2$Cu$_3$O$_{6.54}$ revealed by X-ray diffraction

Charge density wave (CDW) order appears throughout the underdoped high-temperature cuprate superconductors, but the underlying symmetry breaking and the origin of the CDW remain unclear. We use X-ray diffraction to determine the microscopic structure of the CDWs in an archetypical cuprate YBa$_2$Cu$_3$O$_{6.54}$ at its superconducting transition temperature ~60K. We find that the CDWs in this material break the mirror symmetry of the CuO$_2$ bilayers. The ionic displacements in the CDWs have two components, which are perpendicular and parallel to the CuO$_2$ planes, and are out of phase with each other. The planar oxygen atoms have the largest displacements, perpendicular to the CuO$_2$ planes. Our results allow many electronic properties of the underdoped cuprates to be understood. For instance, the CDWs will lead to local variations in the electronic structure, giving an explicit explanation of density-wave states with broken symmetry observed in scanning tunnelling microscopy and soft X-ray measurements.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, University of Birmingham, Universität Zürich, University of Liverpool, University of British Columbia, Deutsches Elektronen-Synchrotron, Brookhaven National Laboratory, University of Bristol
Authors: Forgan, E. (Ekstern), Blackburn, E. (Ekstern), Holmes, A. (Ekstern), Briffa, A. (Ekstern), Chang, J. (Ekstern), Bouchenoire, L. (Ekstern), Brown, S. (Ekstern), Liang, R. (Ekstern), Bonn, D. (Ekstern), Hardy, W. (Ekstern), Christensen, N. B. (Intern), Zimmermann, M. V. (Ekstern), Hücker, M. (Ekstern), Hayden, S. (Ekstern)
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BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 11.8 SJR 6.414 SNIP 2.855
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 6.287 SNIP 2.86 CiteScore 11.23
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
The Next Generation of Axion Helioscopes: The International Axion Observatory (IAXO)

The International Axion Observatory (IAXO) is a proposed 4th-generation axion helioscope with the primary physics research goal to search for solar axions via their Primakoff conversion into photons of 1 – 10 keV energies in a strong magnetic field. IAXO will achieve a sensitivity to the axion-photon coupling gain down to a few $\times 10^{-12}$ GeV$^{-1}$ for a wide range of axion masses up to $\sim 0.25$eV. This is an improvement over the currently best (3rd generation) axion helioscope, the CERN Axion Solar Telescope (CAST), of about 5 orders of magnitude in signal strength, corresponding to a factor $\sim 20$ in the axion photon coupling. IAXO's sensitivity relies on the construction of a large superconducting 8-coil toroidal magnet of 20 m length optimized for axion research. Each of the eight 60cm diameter magnet bores is equipped with x-ray optics focusing the signal photons into $\sim 0.2$cm$^2$ spots that are imaged by very low background x-ray detectors. The magnet will be built into a structure with elevation and azimuth drives that will allow solar tracking for 12 hours each day.

This contribution is a summary of our papers [1–3] and we refer to these for further details.

General information
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Organisations: National Space Institute, Astrophysics, Department of Physics, Neutrons and X-rays for Materials Physics, Lawrence Livermore National Laboratory, Centre d'Etudes Nucléaires de Saclay, University of South Carolina, CERN, University of Trieste, Lawrence Berkeley National Laboratory, Dogus University, Universidad de Zaragoza, University of Haifa
Authors: Vogel, J. (Ekstern), Armengaud, E. (Ekstern), Avignone, F. (Ekstern), Betz, M. (Ekstern), Brax, P. (Ekstern), Brun, P. G. (Ekstern), Cantatore, G. (Ekstern), Carmona, J. (Ekstern), Carosi, G. (Ekstern), Caspers, F. (Ekstern), Caspi, S. (Ekstern), Cetin, S. (Ekstern), Chelouche, D. (Ekstern), Christensen, F. E. (Intern), Jakobsen, A. C. (Intern)
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Scopus rating (2015): SJR 0.262 SNIP 0.572 CiteScore 0.61
Scopus rating (2014): SJR 0.401 SNIP 0.696 CiteScore 0.78
Scopus rating (2013): SJR 0.29 SNIP 0.605 CiteScore 0.72
ISI indexed (2013): ISI indexed no
Theoretical study of time-dependent, ultrasound-induced acoustic streaming in microchannels

Based on first- and second-order perturbation theory, we present a numerical study of the temporal buildup and decay of unsteady acoustic fields and acoustic streaming flows actuated by vibrating walls in the transverse cross-sectional plane of a long straight microchannel under adiabatic conditions and assuming temperature-independent material parameters. The unsteady streaming flow is obtained by averaging the time-dependent velocity field over one oscillation period, and as time increases, it is shown to converge towards the well-known steady time-averaged solution calculated in the frequency domain. Scaling analysis reveals that the acoustic resonance builds up much faster than the acoustic streaming, implying that the radiation force may dominate over the drag force from streaming even for small particles. However, our numerical time-dependent analysis indicates that pulsed actuation does not reduce streaming significantly due to its slow decay. Our numerical time-dependent analysis also shows that for an acoustic resonance with a quality factor Q, the amplitude of the oscillating second-order velocity component is Q times larger than the usual second-order steady time-averaged velocity component.

Consequently, the well-known criterion \( v_1 \ll c_s \) for the validity of the perturbation expansion is replaced by the more restrictive criterion \( v_1 \ll c_s / Q \). Our numerical model is available as supplemental material in the form of comsol model files and matlab scripts.
Thin films of CZTS prepared by Pulsed Laser Deposition

**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, Experimental Surface and Nanomaterials Physics
Authors: Cazzaniga, A. C. (Intern), Ettlinger, R. B. (Intern), Engberg, S. L. J. (Intern), Canulescu, S. (Intern), Crovetto, A. (Intern), Pryds, N. (Intern), Hansen, O. (Intern), Schou, J. (Intern)
Publication date: 2015
Main Research Area: Technical/natural sciences

Electronic versions:
Three-dimensional nanometrology of microstructures by replica molding and large-range atomic force microscopy

We have used replica molding and large-range atomic force microscopy to characterize the three-dimensional shape of high-aspect-ratio microstructures. Casting inverted replicas of microstructures using polydimethylsiloxane (PDMS) circumvents the inability of AFM probes to measure deep and narrow cavities. We investigated cylindrical deep reactive ion etched cavities in silicon wafers and determined the radius of curvature (ROC) of the sidewalls as a function of depth. Statistical analysis verified the reliability and reproducibility of the replication procedure. The mean ROC was determined as \((6.32 \pm 0.06) \text{ nm}\), i.e., with 1% accuracy, while the ROC linearly increases by \((0.52 \pm 0.03) \text{ nm}\) from the top to the bottom of the sidewalls. Nanometer-sized surface defects are also well replicated. In addition, the method allows combining multiple features from differently processed wafers into a single sample, accelerating characterization in process optimization tasks. To access the sidewall shape samples needed to be cleaved. The method was applied to study X-ray refractive optics, whose performance is crucially affected by their three-dimensional shapes.

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Publication: Research - peer-review » Journal article – Annual report year: 2015

**TiO2-Si solar cells with carrier selective contacts and low temperature processing**

General information
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Organisations: Department of Micro- and Nanotechnology, Silicon Microtechnology, Experimental Surface and Nanomaterials Physics
Authors: Plakhotnyuk, M. (Intern), Hansen, O. (Intern)
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Bibliographical note
Poster presentation

Relations
Projects:
TiO2-Si solar cells with carrier selective contacts and low temperature processing
Publication: Research - peer-review » Conference abstract in proceedings – Annual report year: 2015

**Toward an Active and Stable Catalyst for Oxygen Evolution in Acidic Media: Ti-Stabilized MnO2**

Catalysts are required for the oxygen evolution reaction, which are abundant, active, and stable in acid. MnO2 is a promising candidate material for this purpose. However, it dissolves at high overpotentials. Using first-principles calculations, a strategy to mitigate this problem by decorating undercoordinated surface sites of MnO2 with a stable oxide is developed here. TiO2 stands out as the most promising of the different oxides in the simulations. This prediction is experimentally verified by testing sputter-deposited thin films of MnO2 and Ti-MnO2. A combination of electrochemical measurements, quartz crystal microbalance, inductively coupled plasma mass spectrometry measurements, and X-ray photoelectron spectroscopy is performed. Small amounts of TiO2 incorporated into MnO2 lead to a moderate improvement in stability, with only a small decrease in activity. This study opens up the possibility of engineering surface properties of catalysts so that active and abundant nonprecious metal oxides can be used in acid electrolytes.

General information
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Organisations: Department of Physics, Center for Individual Nanoparticle Functionality, Center for Atomic-scale Materials Design, Department of Chemistry
Towards first principles modeling of electrochemical electrode-electrolyte interfaces

We present a mini-perspective on the development of first principles modeling of electrochemical interfaces. We show that none of the existing methods deal with all the thermodynamic constraints that the electrochemical environment imposes on the structure of the interface. We present two directions forward to make the description more realistic and correct. © 2014 Elsevier B.V. All rights reserved.

General information
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Organisations: Theoretical Atomic-scale Physics, Center for Atomic-scale Materials Design, Department of Physics
Authors: Nielsen, M. (Intern), Björketun, M. (Intern), Hansen, M. H. (Intern), Rossmeisl, J. (Intern)
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Scopus rating (2010): SJR 1.228 SNIP 0.858
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Scopus rating (2006): SJR 1.287 SNIP 0.947
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Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 1.401 SNIP 1.049
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 1.812 SNIP 1.041
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Authors: Mogensen, M. B. (Intern), Stephens, I. E. (Intern)
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Tre tigerspring for materialeforskningen

**General information**
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Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Aarhus University, University of Copenhagen
Authors: Willendrup, P. K. (Intern), Jørgensen, M. R. V. (Ekstern), Lefmann, K. (Ekstern), Haldrup, K. (Intern)
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Tunable 1.9μm laser system for Mid-IR upconversion detection

A tunable 1.9μm Tm:YLF laser was built for low noise infrared upconversion imaging and spectroscopy. Its noise properties are compared to that obtained using a 1064nm mixing laser, focusing on spontaneous parametric downconversion generated noise.

**General information**
State: Published
Tuning the Schottky Barrier at the Graphene/MoS2 Interface by Electron Doping: Density Functional Theory and Many-Body Calculations

Using ab initio calculations we investigate the energy level alignment at the graphene/MoS2 heterostructure and the use of electron doping as a strategy to lower the Schottky barrier and achieve a low-resistance Ohmic contact. For the neutral heterostructure, density functional theory (DFT) with a generalized gradient approximation predicts a Schottky barrier height of 0.18 eV, whereas the G0W0 method increases this value to 0.60 eV. While the DFT band gap of MoS2 does not change when the heterostructure is formed, the G0W0 gap is reduced by 0.30 eV as a result of the enhanced screening by the graphene layer. In contrast to the case of metal substrates, where the band alignment is governed by Pauli repulsion-induced interface dipoles, the graphene/MoS2 heterostructure shows only a negligible interface dipole. As a consequence, the band alignment at the neutral heterostructure is not changed when the two layers are brought into contact. We systematically follow the band alignment as a function of doping concentration and find that the Fermi level of the graphene crosses the MoS2 conduction band at a doping concentration of around $10^{12}$ cm$^{-2}$. The variation of the energy levels with doping concentration is shown to be mainly governed by the electrostatic potential resulting from the doping charge.
Two-dimensional metal dichalcogenides and oxides for hydrogen evolution: A computational screening approach

We explore the possibilities of hydrogen evolution by basal planes of 2D metal dichalcogenides and oxides in the 2H and 1T class of structures using the hydrogen binding energy as a computational activity descriptor. For some groups of systems like the Ti, Zr, and Hf dichalcogenides the hydrogen bonding to the 2H structure is stronger than that to the 1T structure, while for the Cr, Mo, and W dichalcogenides the behavior is opposite. This is rationalized by investigating shifts in the chalcogenide p levels comparing the two structures. We find that usually for a given material only at most one of the two phases will be active for the hydrogen evolution reaction; however, in most cases the two phases are very close in formation energy, opening up the possibility for stabilizing the active phase. The study points to many new possible 2D HER materials beyond the few that are already known.
Two level undercut-profile substrate for filamentary YBa$_2$Cu$_3$O$_7$ coated conductors: Fast Track Communication

A novel substrate design is presented for scalable industrial production of filamentary coated conductors (CCs). The new substrate, called ‘two level undercut-profile substrate (2LUPS)’, has two levels of plateaus connected by walls with an undercut profile. The undercuts are made to produce a shading effect during subsequent deposition of layers, thereby creating gaps in the superconducting layer deposited on the curved walls between the two levels. It is demonstrated that
such 2LUPS-based CCs can be produced in a large-scale production system using standard deposition processes, with no additional post-processing. Inspection of the conductor cross-section reveals that the deposited superconducting layer is physically separated at the 2LUPS undercuts. Filament decoupling is also seen in maps of the remanent magnetic field and confirmed by transport measurements.
Uncertainty budget for determinations of mean isomer shift from Mössbauer spectra

General information
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Organisations: Department of Micro- and Nanotechnology, Magnetic Systems, Department of Physics, Neutrons and X-rays for Materials Physics, Royal Institution of Great Britain, Physikalisch-Technische Bundesanstalt
Authors: Fock, J. (Intern), Bogart, L. (Ekstern), Posth, O. (Ekstern), Hansen, M. F. (Intern), Pankhurst, Q. (Ekstern), Frandsen, C. (Intern)
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Use 200x less material! Solar cells based on the Cu2ZnSnS4 compound

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Authors: Crovetto, A. (Intern), Engberg, S. (Intern), Ettlinger, R. (Intern), Cazzaniga, A. (Intern), Schou, J. (Intern), Hansen, O. (Intern)
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Using Protection Layers for a 2-Photon Water Splitting Device

The 2-photon tandem device for photocatalytic water splitting has been theoretically shown to provide a higher efficiency than a single photon device(1). This increased efficiency can be achieved by having one material optimized to absorb high energy photons (large bandgap) and another material optimized to absorb low energy photons (small bandgap). To a large degree this approach has been hindered by corrosion issues. In this talk I will first discuss how our computational screening of 2,400 materials showed that very few materials can efficiently absorb light without corroding in water splitting conditions.(2) I will follow this up by discussing how protection layers bypass the corrosion issue by creating a buffer layer.(3) Finally I will show how we integrated a photocatalyst/protection layer/(co-catalyst) scheme to produce highly efficient H2 evolution photocathodes and O2 evolution photoanodes.(3, 4) 1. A. B. Laursen, S. Kegnaes, S. Dahl and I. Chorkendorff, Energy & Environmental Science, 5 (2012). 2. B. Seger, I. E. Castelli, P. C. K. Vesborg, K. W. Jacobsen, O. Hansen and I. Chorkendorff, Energy & Environmental Science, 7, 2397 (2014). 3. B. Seger, T. Pedersen, A. B. Laursen, P. C. K. Vesborg, O. Hansen and I. Chorkendorff, Journal of the American Chemical Society, 135, 1057 (2013). 4. B. Mei, A. A. Permyakova, R. Frydendal, D. Bae, T. Pedersen, P. Malacrida, O. Hansen, I. E. L. Stephens, P. C. K. Vesborg, B. Seger and I. Chorkendorff, The Journal of Physical Chemistry Letters, 5, 3456 (2014). [Figure]

Valley Hall effect in disordered monolayer MoS2 from first principles

Electrons in certain two-dimensional crystals possess a pseudospin degree of freedom associated with the existence of two inequivalent valleys in the Brillouin zone. If, as in monolayer MoS2, inversion symmetry is broken and time-reversal symmetry is present, equal and opposite amounts of k-space Berry curvature accumulate in each of the two valleys. This is conveniently quantified by the integral of the Berry curvature over a single valley-the valley Hall conductivity. We generalize this definition to include contributions from disorder described with the supercell approach, by mapping ("unfolding") the Berry curvature from the folded Brillouin zone of the disordered supercell onto the normal Brillouin zone of the pristine crystal, and then averaging over several realizations of disorder. We use this scheme to study from first principles the effect of sulfur vacancies on the valley Hall conductivity of monolayer MoS2. In dirty samples the intrinsic valley Hall conductivity receives gating-dependent corrections that are only weakly dependent on the impurity concentration, consistent with side-jump scattering and the unfolded Berry curvature can be interpreted as a k-space resolved side jump. At low impurity concentrations skew scattering dominates, leading to a divergent valley Hall conductivity.
conductivity in the clean limit. The implications for the recently observed photoinduced anomalous Hall effect are discussed.
Velocity-space observation regions of high-resolution two-step reaction gamma-ray spectroscopy

High-resolution γ-ray spectroscopy (GRS) measurements resolve spectral shapes of Dopplerbroadened γ-rays. We calculate weight functions describing velocity-space sensitivities of any two-step reaction GRS measurements in magnetized plasmas using the resonant nuclear reaction \(^9\text{Be}(\alpha, \text{n} \gamma)\text{^{12}C}\) as an example. The energy-dependent cross sections of this reaction suggest that GRS is sensitive to alpha particles above about 1.7 MeV and highly sensitive to alpha particles at the resonance energies of the reaction. Here we demonstrate that high resolution two-step reaction GRS measurements are not only selective in energy but also in pitch angle. They can be highly sensitive in particular pitch angle ranges and completely insensitive in others. Moreover, GRS weight functions allow rapid calculation of γ-ray energy spectra from fast-ion distribution functions, additionally revealing how many photons any given alpha-particle velocity-space region contributes to the measurements in each γ-ray energy bin.

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Velocity-space sensitivity of neutron spectrometry measurements

Neutron emission spectrometry (NES) measures the energies of neutrons produced in fusion reactions. Here we present velocity-space weight functions for NES and neutron yield measurements. Weight functions show the sensitivity as well as the accessible regions in velocity space for a given range of the neutron energy spectrum. Combined with a calculated fast-ion distribution function, they determine the part of the distribution function producing detectable neutrons in a given neutron energy range. Furthermore, we construct a forward model based on weight functions capable of rapidly calculating neutron energy spectra. This forward model can be inverted and could thereby be used to directly measure the fast-ion phase-space distribution functions, possibly in combination with other fast-ion diagnostics. The presented methods and results can be applied to neutron energy spectra measured by any kind of neutron spectrometer and to any neutron yield measurement.
Visualizing the non-equilibrium dynamics of photoinduced intramolecular electron transfer with femtosecond X-ray pulses

Ultrafast photoinduced transient optical absorption spectroscopy with ultrafast X-ray emission spectroscopy and diffuse X-ray scattering at the SACLA facility to track the non-equilibrated electronic and structural dynamics within a bimetallic donor–acceptor complex that contains an optically dark centre. Exploiting the 100-fold increase in temporal resolution as compared with storage ring facilities, these measurements constitute the first X-ray-based visualization of a non-equilibrated intramolecular electron transfer process over large interatomic distances. Experimental and theoretical results establish that mediation through electronically excited molecular states is a key mechanistic feature. The present study demonstrates the extensive potential of femtosecond X-ray techniques as diagnostics of non-adiabatic electron transfer processes in synthetic and biological systems, and some directions for future studies, are outlined.

General information
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Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Center for Atomic-scale Materials Design, Department of Chemistry, Physical and Biophysical Chemistry, Lund University, University of Copenhagen, Hungarian Academy of Sciences, High Energy Accelerator Research Organization, The Hamburg Centre for Ultrafast Imaging, European XFEL, Argonne National Laboratory, The Institute of Chemical and Physical Research, Japan Synchrotron Radiation Research Institute
Number of pages: 10
Publication date: 2015
Main Research Area: Technical/natural sciences
What Is the Optimum Strain for Pt Alloys for Oxygen Electroreduction?

In order to make low-temperature fuel cells commercially viable, it is crucial to develop oxygen reduction catalysts based on more active, stable and abundant materials. A fruitful strategy for enhancing the oxygen reduction reaction (ORR) activity is to alloy Pt with transition metals [1]. However, commercial alloys of Pt and late transition metals such as Ni, Co or Fe are typically unstable under fuel-cell conditions [2]. The very negative enthalpy of formation of alloys of Pt and lanthanides could provide them with greater long term stability than Pt and late transition metals. Herein, we show the trends in activity and stability novel Pt-lanthanide (Pt-Ln) alloys as efficient ORR catalysts. Sputter-cleaned, polycrystalline Pt5Gd shows a 5-fold increase in ORR activity [3], relative to Pt. All the Pt-lanthanide alloys are at least 3 times more active than Pt for the ORR [3-5]. A compressed Pt overlayer is formed onto the bulk alloy. Accordingly, the effect of alloying Pt is to impose strain onto the Pt overlayer [3-5]. It is likely that this strain would be relaxed by defects [6]. The lattice parameter is presented as a new descriptor that controls both the activity and stability of these materials [5]. The best performance (activity-stability) is achieved by Pt5Gd. Furthermore, mass-selected PtxGd nanoparticles synthesised by the gas aggregation technique present a significant ORR activity enhancement as compared to pure Pt nanoparticles, PtxGd 8 nm showing 3.6 A (mg Pt)-1 mass activity (Fig. 1B) [7], surpassing the highest activity reached with PtxY nanoparticles [8]. The activity of PtxGd nanoparticles also correlates strongly with compressive strain. Our results demonstrate that we can engineer both the activity and stability by tuning the Pt-Pt distance. References [1] I.E.L. Stephens, A.S. Bondarenko, U. Grønbjerg, J. Rossmeisl, I. Chorkendorff, Energy Environ. Sci. 2012, 5, 6744. [2] S. Chen, H.A. Gasteiger, K. Hayakawa, T. Tada, Y. Shao-Horn, J. Electrochem. Soc. 2010, 1571, A82. [3] M. Escudero-Escribano, et al., J. Am. Chem. Soc. 2012, 130, 16476. [4] P. Malacrida, M. Escudero-Escribano, A. Verdaguer-Casadevall, I.E.L. Stephens, I. Chorkendorff, J. Mater. Chem. A 2014, 2, 4234. [5] M. Escudero-Escribano, et al., to be submitted, 2014. [6] P. Strasser, et al., Nature Chem. 2010, 2, 454. [7] A. Velázquez-Palenzuela, et al., J. Catal., accepted, 2014. [8] P. Hernandez-Fernandez, et al., Nature Chem. 2014, 6, 732. Fig 1. (A) ORR kinetic current density as a function of the lattice parameter and the Pt-Pt distance for Pt5Ln and Pt. (B) Mass activity of PtxGd, PtxY and Pt nanoparticles. All activity values were taken at 0.9 V vs. RHE, from cyclic voltammetry recorded at 50 mV s-1 and 1600 rpm in O2-saturated 0.1M HClO4. [Figure]
We present insights into the mechanism and the active site for hydrogen evolution on nickel phosphide (Ni2P). Ni2P was recently discovered to be a very active non-precious hydrogen evolution catalyst. Current literature attributes the activity of Ni2P to a particular site on the (0001) facet. In the present study, using Density Functional Theory (DFT) calculations, we show that several widely available low index crystal facets on Ni2P have better properties for a high catalytic activity. DFT calculations were used to identify moderately bonding nickel bridge sites and nickel hollow sites for hydrogen adsorption and to calculate barriers for the Tafel pathway. The investigated surfaces in this study were the (101) over bar0, (112) over bar0, (112) over bar1 and (0001) facets of the hexagonal Ni2P crystal. In addition to the DFT results, we present experiments on Ni2P nanowires growing along the <0001 > direction, which are shown as efficient hydrogen evolution catalysts. The experimental results add these nanowires to a variety of different morphologies of Ni2P, which are all active for HER.
ZnS top layer for enhancement of the crystallinity of CZTS absorber during the annealing

Pulsed Laser Deposition (PLD) of thin films of Cu2ZnSnS4 (CZTS) has not yet led to solar cells with high efficiency. The reason for the relative low efficiency is discussed and a way to overcome this issue is presented. The present thin film absorbers of CZTS suffer from loss of volatile Zn during the plasma-assisted transfer with PLD. This can be compensated by adding a thin layer of ZnS (∼ 80 nm) on top of the CZTS layer before the annealing. In this work the stack ordering of
the two layers CZTS and ZnS is investigated, indicating that the configuration with ZnS on top of a CZTS film gives a better crystalline quality of CZTS after the annealing, as demonstrated by X-ray diffraction and Raman spectroscopy.

**General information**
- **State:** Published
- **Organisations:** Department of Photonics Engineering, Optical Microsensors and Micromaterials, Department of Micro- and Nanotechnology, Silicon Microtechnology, Risø National Laboratory for Sustainable Energy, Department of Physics, Experimental Surface and Nanomaterials Physics, Department of Energy Conversion and Storage, Electrofunctional materials
- **Authors:** Cazzaniga, A. C. (Intern), Crovetto, A. (Intern), Ettlinger, R. B. (Intern), Canulescu, S. (Intern), Hansen, O. (Intern), Pryds, N. (Intern), Schou, J. (Intern)
- **Number of pages:** 4
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- **Source:** Findit
- **Source-ID:** 276914239
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**Zooplankton Hydrodynamics: An investigation into the physics of aquatic interactions**

Zooplankton are hugely abundant organisms found in all aquatic environments and form an important part of the marine ecosystems. Most zooplankton swim in order to find food and mates, and to avoid predators. In spite of its advantages, swimming comes with trade-offs, it costs energy and creates flow disturbances that may attract predators. The first part of this thesis attempts to quantify the trade-offs associated with the swimming behaviour of diverse zooplankton.

We measured the swimming kinematics and flow fields around the 'jumping' copepod Acartiia tonsa at various stages of its life cycle, and found qualitative differences in flow structures, energy expenditure, and swimming efficiency, between the early and later stages. The spatial decay rate of flow disturbances was faster in the later stages, suggesting that those may be less vulnerable to predation. Broadening the scope, we then measured flows around a wide range of zooplankton which use a variety of swimming modes such as hovering, cruising, jumping, and breast stroke swimming. We found that the spatial decay rate of the flow velocity is dictated by the swimming mode. The modes used for swimming only, such as jumping and breast stroke swimming, had much faster spatial decay as compared to the other modes, resulting in 'quiet' swimming.

This motivated us to examine breast stroke swimming in more detail, for which flow velocity decayed spatially as one over distance cubed. We employed a simple model using three point forces to represent the forces acting on the swimmer. Our analysis showed a configuration-dependent spatial decay of flow velocity. Arranging the propulsive forces close to the equator resulted in changing the far field velocity decay from one over distance squared to one over distance cubed, comparing well with the experimental observations. To further investigate periodic swimming using breast stroke, we measured detailed swimming dynamics and induced flows for the cladoceran Podon intermedius. We estimated the propulsive forces acting on P. intermedius, which showed that the fast spatial decay in the induced flows was not explained by the three point force model. We speculate that this is due to inertial effects in the flow, which seem to play an important role in the swimming of larger zooplankton. We also developed a simple model to mimic the dynamics of periodic swimming, which showed that non-linear drag terms are needed in the model to correctly capture the observed dynamics.

The second part of this thesis examines how size dictates transitions in life strategies, and thus acts as a structuring factor in marine life. To this end, we reviewed data on size-based scaling laws for resource acquisition, motility, sensing, and offspring size for all pelagic marine life, from bacteria to whales. We also reviewed and developed theoretical arguments for the observed scaling laws and for the characteristic sizes at which transitions from one strategy to another take place. Based on our findings, we divided life in the ocean into seven major realms based on trophic strategy, physiology, and life history strategy.

Finally, we delve deeper into size based structuring of sensory strategies in the ocean. Survival in the open ocean requires effective collection of information from the surroundings via the use of various sensory modes. We studied how sensing modes and their respective ranges depend on body size. We investigated the physiological constraints on sense organs, together with the physics of signal generation, transmission, and reception. Our analysis revealed a hierarchy of sensing modes - with increasing size, a larger battery of sensory modes becomes available and the sensing range increases. Our
theoretical predictions of lower and upper size limits for various senses aligned well with the size ranges found in the literature. Although the scaling analyses and the size limits are only first order estimates, this work forms the first comprehensive analysis of the size based structuring of sensory modes used by marine life.

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Collapsible Photovoltaic Module for a Large-Scale Solar Power Plant
An elongate photovoltaic (PV) module for use in a solar energy conversion plant for the production of electricity from incident light, the PV-module comprising a top portion with a support panel (G) carrying on a front side a plurality of electrically connected PV cells (D), and a transparent protective layer (A) sealed to the support panel (G) so as to encapsulate the PV-cells (D) between the support panel (G) and the protective layer (A), wherein prior to installation of the PV-module at the deployment site a collapsible portion of the PV-module is configured to be collapsible in a longitudinal direction by folding and/or rolling, wherein the collapsible portion includes at least the top portion, wherein the PV-module further comprises one or more integrated ballast chambers (I) in a bottom portion of the PV-module arranged on a rear side of the support panel (G), wherein said integrated ballast chamber (I) after installation of the PV-module at the deployment site contains an amount of a ballasting material (H) with a weight sufficient to immobilize the PV-module on a supporting surface of the deployment site under predetermined characteristic climate conditions for the deployment site.

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Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics
Authors: Vesborg, P. C. K. (Intern)
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Source: espacenet
Source-ID: US2014238464
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2-Photon tandem device for water splitting: comparing photocathode first versus photoanode first designs
Within the field of photocatalytic water splitting there are several strategies to achieve the goal of efficient and cheap photocatalytic water splitting. This work examines one particular strategy by focusing on monolithically stacked, two-photon photoelectrochemical cells. The overall aim of the analysis is to compare the relative merits of two fundamentally different designs: one, where the photoanode is the large bandgap material (light-facing side), and the other, where the photocathode is the large bandgap material. Even though the former design is often shown in the literature, the present analysis shows that the latter design has several advantages. This is particularly true when considering designs that incorporate protection layers to protect the photoabsorbers. A high throughput computational screening was used to filter materials databases in search of candidates with the correct properties. These results show that without protective layers
there are scarcely any materials which seem viable as photoabsorbers whereas with protection layers there are significantly more candidates. Since the protection layer (and redox catalysts) on the light facing side should not interfere with light absorption, this is the more difficult side to optimize. Nevertheless, by using TiO2 as a transparent cathode protection layer in conjunction with known H-2 evolution catalysts, protection is clearly feasible for a large bandgap photocathode. This suggests that there may be promising strategies for photocatalytic water splitting by using a large bandgap photocathode and a low bandgap photoanode with attached protection layers.
3D-Ray Diffraction Microscopy

Three-dimensional X-ray diffraction (3DXRD) microscopy is a fast and non-destructive structural characterization technique aimed at the study of individual crystalline elements (grains or subgrains) within mm-sized polycrystalline specimens. It is based on two principles: the use of highly penetrating hard X-rays from a synchrotron source and the application of “tomographic” reconstruction algorithms for the analysis of the diffraction data. In favorable cases, the position, morphology, phase, and crystallographic orientation can be derived for up to a thousand elements simultaneously. For each grain its average strain tensor may also be derived, from which the type-II stresses can be inferred. Furthermore, the dynamics of the individual elements can be monitored during typical processes such as deformation or annealing. Hence, information on the interaction between elements can be obtained directly. In this chapter we first provide an overview of the various experimental approaches for 3DXRD that have emerged. Following this, a more detailed presentation of work related to the classical 3DXRD setup is given. Some emphasis is also placed on the mathematical challenges inherent to the reconstruction of grain and orientation maps.

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3D Simulations of Plasma Filaments in the Scrape Off Layer

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Ab Initio Thermodynamic Modeling of Electrified Metal–Oxide Interfaces: Consistent Treatment of Electronic and Ionic Chemical Potentials

Solid oxide fuel cells are attractive devices in a sustainable energy context because of their fuel flexibility and potentially highly efficient conversion of chemical to electrical energy. The performance of the device is to a large extent determined by the atomic structure of the electrode–electrolyte interface. Lack of atomic-level information about the interface has limited the fundamental understanding, which further limits the opportunity for optimization. The atomic structure of the interface is affected by electrode potential, chemical potential of oxygen ions, temperature, and gas pressures. In this paper we present a scheme to determine the metal–oxide interface structure at a given set of these environmental parameters based on quantum chemical calculations. As an illustration we determine the structure of a Ni-YSZ anode as a function of electrode potential at 0 and 1000 K. We further describe how the structural information can be used as a starting point for accurate calculations of the kinetics of fuel oxidation reactions, in particular the hydrogen oxidation reaction. More generally, we anticipate that the scheme will be a valuable theoretical tool to describe solid–solid electrochemical interfaces.
Accurate Ground-State Energies of Solids and Molecules from Time-Dependent Density-Functional Theory

We demonstrate that ground-state energies approaching chemical accuracy can be obtained by combining the adiabatic-connection fluctuation-dissipation theorem with time-dependent density-functional theory. The key ingredient is a renormalization scheme, which eliminates the divergence of the correlation hole characteristic of any local kernel. This new class of renormalized kernels gives a significantly better description of the short-range correlations in covalent bonds compared to the random phase approximation (RPA) and yields a fourfold improvement of RPA binding energies in both molecules and solids. We also consider examples of barrier heights in chemical reactions, molecular adsorption, and graphene interacting with metal surfaces, which are three examples where the RPA has been successful. In these cases, the renormalized kernel provides results that are of equal quality or even slightly better than the RPA, with a similar computational cost.
Acoustic interaction forces between small particles in an ideal fluid

We present a theoretical expression for the acoustic interaction force between small spherical particles suspended in an ideal fluid exposed to an external acoustic wave. The acoustic interaction force is the part of the acoustic radiation force
on one given particle involving the scattered waves from the other particles. The particles, either compressible liquid droplets or elastic microspheres, are considered to be much smaller than the acoustic wavelength. In this so-called Rayleigh limit, the acoustic interaction forces between the particles are well approximated by gradients of pair-interaction potentials with no restriction on the interparticle distance. The theory is applied to studies of the acoustic interaction force on a particle suspension in either standing or traveling plane waves. The results show aggregation regions along the wave propagation direction, while particles may attract or repel each other in the transverse direction. In addition, a mean-field approximation is developed to describe the acoustic interaction force in an emulsion of oil droplets in water.

**General information**

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The focus of this Ph.D. thesis is on the electrocatalytic oxygen evolution reaction (OER) in acidic media for Proton Exchange Membrane (PEM) Electrolyser applications. This technology is an attractive alternative for storage of renewable energy, such as from solar and wind power, in small scale delocalized hydrogen refueling stations. The sluggish kinetics of OER and the high costs of the materials represent some of the biggest technological challenges for PEM electrolysers. The current technology relies on Pt group based materials and in particular ruthenium and iridium are the most active and stable OER catalysts. To contain costs and precious metals supply, the mass activity should be maximized. However, in order to define the properties of a catalyst, knowing the distinction between geometric and electronic effects is fundamental.

It is not trivial to determine the intrinsic catalytic activity on oxides and studies on well-defined surfaces are required. Notably, industrial applications demand maximized surface-to-bulk ratio, hence fabrication of catalysts in nanoparticulate form. In this perspective, this project aimed at investigating well-defined mass-selected ruthenium and ruthenium dioxide nanoparticles (NPs) in the technological relevant size range of 2-9 nm. The objectives were to estimate the intrinsic catalytic activity of ruthenium and to identify any particle size effects. The results show that activity and stability are strongly influenced by the surface pre-treatment. Furthermore, these RuO₂ NPs exhibit over an order of magnitude improvement in activity and turnover frequency in comparison to the current state-of-the-art, and a tentative maximum at around 3-5 nm.

Although high activity is essential for an efficient catalyst, stability should be also considered, in particular under the harsh acidic and oxidizing conditions for a PEM electrolyser. Standardised protocols for assessing the stability have not been established for the oxygen evolution reaction. Hence, this thesis focuses on providing guidelines for quantifying the corrosion rate of an OER catalyst. By coupling Electrochemical Quartz Crystal Microbalance (EQCM) measurements with Inductively Coupled Plasma – Mass Spectrometry (ICP-MS) analyses of the electrolyte, we emphasize the importance of monitoring the mass loss.

Finally, the thesis focuses on improving the stability of ruthenium dioxide under OER conditions, by sub-monolayer addition of iridium oxide. The approach was inspired by theoretical calculations, which suggested that iridium would impede Ru corrosion by migrating to the undercoordinated sites at the surface, such as step and kink sites, which are the most prone to corrosion. Preliminary results show that an improvement of stability can be obtained, slightly decreasing the activity as well. Unfortunately, a drastic enhancement, as hoped, was not detected. Instead the results serve as a starting point from which the strategy and method for stability improvements can be further developed.
Adding the Environmental TEM to the In Situ Toolbox for Catalyst Characterization

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Adsorbate induced surface alloy formation investigated by near ambient pressure X-ray photoelectron spectroscopy
Formation of meta-stable surface-alloys can be used as a way to tune the binding strength of reaction intermediates and could therefore be used as improved catalyst materials for heterogeneous catalysis. Understanding the role of adsorbates on such alloy surfaces can provide new insights for engineering of more active or selective catalyst materials. Dynamical surface changes on alloy surfaces due to the adsorption of reactants in high gas pressures are challenging to investigate using standard characterization tools. Here we apply synchrotron illuminated near ambient pressure X-ray photoelectron spectroscopy to probe the surface structure of a CuPt model system. We report an investigation of the formation of a CuPt surface alloy induced and stabilized by exposure to mbar pressures of CO. The location of Pt within the alloy is assessed by deconvolution of the Pt 4f core level spectra into surface Pt and bulk Pt contributions. The study provides direct evidence on how it is possible to monitor the surface structure under near operation conditions. © 2014 Elsevier B.V. All rights reserved.

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Advanced dry etching studies for micro- and nano-systems

Dry etching is a collective term used for controlled material removal by means of plasma generated ions. Dry etching includes several techniques, with reactive ion etching as one of the most used of its many derivatives. In this work inductively coupled plasma reactive ion etching has been applied for structuring of sapphire and many polymers. Metals and metal alloys have been structured by physical sputtering with argon ions in an ion beam etching system. The materials for which etch characteristics have been investigated are commonly used in device fabrication at DTU-Danchip. Ion beam etching was first used for structuring of a magnetic device containing four different materials in nine layers. The materials, tantalum, tantalum oxide, iridium-manganese, and permalloy, can all be etched by reactive ion etching, however the thin layers and the need to etch all layers in one process makes ion beam etching an ideal choice. The physical nature of ion beam etching ensures etch rates of the different layers to only differ slightly, however, the etch rate is low. One problem with this technique can be redeposition of etched material at the sidewalls and at resist walls. This can introduce short circuits and even contaminate the surface with metal flakes after resist removal. Ion beam etching has also been used for etching of steel without any problems with redeposition. For steel the etch rate was low which reduced the...
selectivity to the photo resist.

Sapphire, a crystal of aluminum oxide, has a very low sputter rate limiting the applicability of ion beam etching. Structuring of sapphire is however interesting for fabrication of prepatterned substrates for gallium nitride epitaxial growth, among others. Such a substrate needs a certain structure height which can be obtained by introducing reactive ion beam etching in a boron trichloride plasma. The etch rates of sapphire in such a plasma can be up to a hundred times faster than rates in ion beam etching. The anisotropy of the etch can be controlled by changing the plasma conditions and fabrication of sloped sidewalls can be achieved.

Reactive ion etching of polymers can be used for several purposes, such as polymer removal, surface properties alternation, or polymer structuring. For material removal any polymer can be etched in an oxygen plasma, including all the polymers used in this project, which include, SU-8, TOPAS®, PLLA, PCL, and PMMA. However, just generating an oxygen plasma does not result in a controllable etch and may give rise to a poor surface for later use. It may be necessary to introduce other gases such as SF6 to reduce surface roughness. Roughness can also be introduced by the mask in the form of redeposition of material on the surface. Since photo resist is a polymer the selectivity is inherently low and a hard mask below is a solution to increase selectivity. Nevertheless great controllability with many shared properties can be achieved for polymer etching in reactive ion etching.

Advanced sources and optical components for the McStas neutron scattering instrument simulation package

We present new McStas components Virtual_mcnp_input and Virtual_tripoli4_input, Virtual_mcnp_output and Virtual_tripoli_output to be used as interface for the MCNP and Tripoli neutron transport codes. Similarly, the new Lens component can be used to describe any refracting material set-up, including lenses and prisms. A new library for McStas adds the ability to describe any geometrical arrangement as a set of polygons. This feature has been implemented in most sample scattering components such as Single_crystal, Incoherent, Isotropic_Sqw (liquids/amorphous/powder), PowderN as well as in Guide_anyshape component for reflecting or absorbing complex set-up. The PSD_Detector component models a neutron absorbing gas volume, taking into account for instance the penetration depth and the associated parallax effect, the charge cloud generated at the absorption location. This gas volume can be enclosed in a scattering material in order to model the absorption and scattering in the detector housing, prior to the actual detection. An extended model of the IN5b time-of-flight spectrometer at the Institut Laue Langevin is used to simulate vanadium and powder diffractograms, making use of the gas detector component.

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Aggregation-induced growth and transformation of β-FeOOH nanorods to micron-sized α-Fe₂O₃ spindles

Intimate interconnection of crystal growth, (oriented) aggregation and phase transformation seem common in the formation of nano-and microcrystalline materials from solutions. Yet, the mechanistic linkages between the different processes have not been fully understood. In this work, we studied the hydrothermal growth of akaganeite (beta-FeOOH) nanorods and their transformation to micron-sized hematite (alpha-Fe₂O₃) spindles using high-resolution cryogenic transmission electron microscopy (cryo-TEM). Only akaganeite particles and hematite spindles were detected in the samples. Further, cryo-electron 3D tomograms show that akaganeite nanorods were aggregated into loose three-dimensional networks with some embedded hematite spindles. Based on our cryo-TEM and additional X-ray diffraction, electron microscopy, and chemical data, we propose the following mechanism: first, formation of the early-stage hematite spindles is driven by phase stability change due to increase in size caused by oriented aggregation of akaganeite. Then, akaganeite particles continue to transform to hematite upon contact with and recrystallization onto hematite surfaces, making hematite grow with a constant aspect ratio and forming micronsized nano-porous single-crystal spindles. Our growth model interprets experimental observations well and it resolves previous long-time debate over whether the hematite spindles are formed via classical Ostwald ripening or by oriented aggregation of hematite nanoparticles. Possibly, this aggregation-based concurrent growth and transformation model may also be applicable to crystal growth and phase transformation in other systems.
All-optical pressure sensor
The present invention relates to an all-optical pressure sensor comprising a waveguide accommodating a distributed Bragg reflector. Pressure sensing can then be provided by utilizing effective index modulation of the waveguide and detection of a wavelength shift of light reflected from the Bragg reflector. Sound sensing may also be provided thereby having an all-optical microphone. One embodiment of the invention relates to an optical pressure sensor comprising at least one outer membrane and a waveguide, the waveguide comprising at least one core for confining and guiding light, at least one distributed Bragg reflector located in said at least one core, and at least one inner deflecting element forming at least a part of the core, wherein the pressure sensor is configured such that the geometry and/or dimension of the at least one core is changed when the at least one outer membrane is submitted to pressure.

Alloy catalyst material
The present invention relates to a novel alloy catalyst material for use in the synthesis of hydrogen peroxide from oxygen and hydrogen, or from oxygen and water. The present invention also relates to a cathode and an electrochemical cell comprising the novel catalyst material, and the process use of the novel catalyst material for synthesising hydrogen peroxide from oxygen and hydrogen, or from oxygen and water.

Alloys of Pt and Rare Earths for the Oxygen Electroreduction Reaction
This thesis presents the development and characterization of a new class of Pt alloys for catalyzing the Oxygen Reduction Reaction (ORR), in perspective of a future substitution of traditional Pt-based catalysts at the cathode of Polymer
Electrolyte Membrane Fuel Cells (PEMFCs). Focused on spectroscopic techniques such as Angle-Resolved X-Ray Photoelectron Spectroscopy (AR-XPS), Ambient Pressure X-Ray Photoelectron Spectroscopy (AP-XPS) and Ion Scattering Spectroscopy (ISS), it takes part in a broader context of studies pursuing the combination of these physical techniques with electrocatalysis. A number of bimetallic alloys based on Pt and a rare earth, like the Pt-Y system or more recently proposed Pt-lanthanide phases, have been tested and characterized.

Polycrystalline Pt5La and Pt5Ce exhibited more than a factor of 3 enhancement in specific activity relative to state-of-the-art polycrystalline Pt. They maintain at least 90% of this activity after accelerated stability tests (10 000 cycles between 0.6 and 1.0 V vs. the Reversible Hydrogen Electrode (RHE) in 0.1 M HClO4 electrolyte). A combination of AR-XPS and ISS measurements allowed to elucidate the active surface phase and structure of these materials, consisting of a ~1 nm thick pure Pt overlayer on top of the bulk alloy, the stable overlayer providing kinetic stability against further dissolution of the lanthanides. We hypothesize that this high stability is related to the very negative heat of formation of their intermetallic phases, that would prevent La and Ce diffusion to the surface. For this structure only strain effects can explain the activity enhancement.

Other alloys of the same class (e.g. Pt5Gd and Pt5Tb) exhibit even higher specific activities, up to 6 times the one of polycrystalline Pt in the case of Pt5Tb, a record activity among polycrystalline alloys. On the basis of their similar crystal structures, the ORR activity of this class of alloys is correlated to the lattice parameter of the bulk, which is expected to define the Pt-Pt distance in the overlayer. The compression of this Pt-Pt distance in the overlayer originates a volcano-shape trend in activity. However, the most active alloys experience higher activity losses during stability tests, suggesting that high levels of compression might not favour the long-term stability of the Pt overlayers. This hypothesis is supported by Density Functional Theory (DFT) calculations and by AR-XPS. A model for the quantitative estimate of the Pt overlayer thickness from AR-XPS measurements indicates a correlation between the thickening of the Pt overlayers and the activity losses, supporting the concept that more compressed overlayers have lower physical stability.

The application of these materials in a fuel cell requires the fabrication in nanoparticulate form. Through the combination of a gas aggregation technique and a time-of-flight mass spectrometer size-selected Pt-Y nanoparticles are produced. With a mass activity of 3.05 A mg-1Pt at 0.9 V vs. RHE, 9 nm Pt-Y nanoparticles are among the most active ORR catalysts ever reported, although they lose 37 % of this activity after stability test. Similar to the case of polycrystals, after immersion in the acidic electrolyte and testing the active phase consists of a Pt shell surrounding an alloyed core. Also in this case the compressed Pt-Pt distance explains the ORR activity enhancement of these catalysts.

The deposition of these 9 nm Pt-Y nanoparticles on the cathode side of a Membrane Electrode Assembly (MEA), part of a specifically prepared fuel cell, allows AP-XPS measurements under operation conditions. As a consequence of potential cycling, Y oxidizes due to the dealloying process which is observed in-situ. The adsorbed species can be also probed and correlated to the electrochemical potential. Near the open circuit potential (OCP) conditions the oxygenated species consist, to a good extent, of non-hydrated OH, similar to the case of pure Pt nanoparticles.

A mixed SOC-turbulence model for nonlocal transport and Lévy-fractional Fokker–Planck equation

The phenomena of nonlocal transport in magnetically confined plasma are theoretically analyzed. A hybrid model is proposed, which brings together the notion of inverse energy cascade, typical of drift-wave- and two-dimensional fluid turbulence, and the ideas of avalanching behavior, associative with self-organized critical (SOC) behavior. Using statistical arguments, it is shown that an amplification mechanism is needed to introduce nonlocality into dynamics. We obtain a consistent derivation of nonlocal Fokker-Planck equation with space-fractional derivatives from a stochastic Markov process with the transition probabilities defined in reciprocal space. The hybrid model observes the Sparre Andersen universality and defines a new universality class of SOC. (C) 2014 Elsevier B.V. All rights reserved.
An Integrated Photoelectrochemical-Chemical Loop for Solar-Driven Overall Splitting of Hydrogen Sulfide

Abundant and toxic hydrogen sulfide (H2S) from industry and nature has been traditionally considered a liability. However, it represents a potential resource if valuable H-2 and elemental sulfur can be simultaneously extracted through a H2S splitting reaction. Herein a photochemical-chemical loop linked by redox couples such as Fe2+/Fe3+ and I-/I-3(-) for photoelectrochemical H-2 production and H2S chemical absorption redox reactions are reported. Using functionalized Si as photoelectrodes, H2S was successfully split into elemental sulfur and H-2 with high stability and selectivity under simulated solar light. This new conceptual design will not only provide a possible route for using solar energy to convert H2S into valuable resources, but also sheds light on some challenging photochemical reactions such as CH4 activation and CO2 reduction.
An Open-Source Data Storage and Visualization Back End for Experimental Data

In this article, a flexible free and open-source software system for data logging and presentation will be described. The system is highly modular and adaptable and can be used in any laboratory in which continuous and/or ad hoc measurements require centralized storage. A presentation component for the data back end has furthermore been written that enables live visualization of data on any device capable of displaying Web pages. The system consists of three parts: data-logging clients, a data server, and a data presentation Web site. The logging of data from independent clients leads to high resilience to equipment failure, whereas the central storage of data dramatically eases backup and data exchange. The visualization front end allows direct monitoring of acquired data to see live progress of long-duration experiments. This enables the user to alter experimental conditions based on these data and to interfere with the experiment if needed. The data stored consist both of specific measurements and of continuously logged system parameters. The latter is crucial to a variety of automation and surveillance features, and three cases of such features are described: monitoring system health, getting status of long-duration experiments, and implementation of instant alarms in the event of failure. © 2013 Society for Laboratory Automation and Screening.

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Application of the MCNPX-McStas interface for shielding calculations and guide design at ESS

Recently, an interface between the Monte Carlo code MCNPX and the neutron ray-tracing code MCNPX was developed [1, 2]. Based on the expected neutronic performance and guide geometries relevant for the ESS, the combined MCNPX-McStas code is used to calculate dose rates along neutron beam guides. The generation and moderation of neutrons is simulated using a full scale MCNPX model of the ESS target monolith. Upon entering the neutron beam extraction region, the individual neutron states are handed to McStas via the MCNPX-McStas interface. McStas transports the neutrons through the beam guide, and by using newly developed event logging capability, the neutron state parameters corresponding to un-reflected neutrons are recorded at each scattering. This information is handed back to MCNPX where it serves as neutron source input for a second MCNPX simulation. This simulation enables calculation of dose rates in the vicinity of the guide. In addition the logging mechanism is employed to record the scatterings along the guides which is exploited to simulate the supermirror quality requirements (i.e. m-values) needed at different positions along the beam guide to transport neutrons in the same guide/source setup.
Application of the MCNPX-McStas interface for shielding calculations at ESS

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A spherical x-ray transform and hypercube sections
We investigate the problem of sampling a unit great circle on the unit sphere $S^3$ as a support of orientation distribution functions on which acts the discrete spherical x-ray transform. The circle's partition subsets are gnomically mapped onto lines that constitute a convex polygon inside the bounding cubes of hypercube. Thus the problem of the great circle tracing is reduced to the problem of the four-dimensional cube sectioning by the plane containing the circle and the intersection figure (the polygon) vertices finding. In this paper, a fast, non-combinatorial approach for the polygon tracing within the general multi-dimensional frame is proposed.

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Assessing the reliability of calculated catalytic ammonia synthesis rates

We introduce a general method for estimating the uncertainty in calculated materials properties based on density functional theory calculations. We illustrate the approach for a calculation of the catalytic rate of ammonia synthesis over a range of transition-metal catalysts. The correlation between errors in density functional theory calculations is shown to play an important role in reducing the predicted error on calculated rates. Uncertainties depend strongly on reaction conditions.
and catalyst material, and the relative rates between different catalysts are considerably better described than the absolute rates. We introduce an approach for incorporating uncertainty when searching for improved catalysts by evaluating the probability that a given catalyst is better than a known standard.
The programme of the Research Unit of the Fusion Association Euratom – DTU, Technical University of Denmark covers work in fusion plasma physics and in fusion technology. The fusion plasma physics research focuses on turbulence and transport, and its interaction with the plasma equilibrium and particles. The effort includes both first principles based modelling, and experimental observations of turbulence and of fast ion dynamics by collective Thomson scattering. Within fusion technology there are activities on fusion materials research (Tungsten and ODSFS). Other activities are system analysis, initiative to involve Danish industry in ITER contracts and public information. A summary is presented of the results obtained in the Research Unit during 2013.

General information
State: Published
Organisations: Department of Physics, Plasma Physics and Fusion Energy
Publication date: 2014

Publication information
Publisher: Department of Physics, Technical University of Denmark
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
Source: PublicationPreSubmission
Source-ID: 100182563
Publication: Research › Report – Annual report year: 2014

A strong steric hindrance effect on ground state, excited state, and charge separated state properties of a CuI-diimine complex captured by X-ray transient absorption spectroscopy
Photophysical and structural properties of a CuI diimine complex with very strong steric hindrance, [Cu(dppS)2]+ (dppS = 2,9-diphenyl-1,10-phenanthroline disulfonic acid disodium salt), are investigated by optical and X-ray transient absorption (OTA and XTA) spectroscopy. The bulky phenylsulfonic acid groups at 2,9 positions of phenanthroline ligands force the ground state and the metal-to-ligand charge-transfer (MLCT) excited state to adopt a flattened pseudo-tetrahedral coordination geometry in which the solvent access to the copper center is completely blocked. We analyzed the MLCT state dynamics and structures as well as those of the charge separated state resulting from the interfacial electron injection from the MLCT state to TiO2 nanoparticles (NPs). The OTA results show the absence of the sub-picosecond component previously assigned as the time constant for flattening, while the two observed time constants are assigned to a relatively slow intersystem crossing (ISC) rate (13.8 ps) and a decay rate (100 ns) of the [Cu(dppS)2]+ MLCT state in water. These results correlate well with the XTA studies that resolved a flattened tetrahedral Cu(i) coordination geometry.
in the ground state. Probing the 3MLCT state structure with XTA establishes that the 3MLCT state has the same oxidation state as the copper center in [CuI(dppS)2]+ and the Cu-N distance is reduced by 0.06 Å compared to that of the ground state, accompanied by a rotation of phenyl rings located at 2,9 positions of phenanthroline. The structural dynamics of the photoinduced charge transfer process in the [CuI(dppS)2]+/TiO2 hybrid is also investigated, which suggests a more restricted environment for the complex upon binding to TiO2 NPs. Moreover, the Cu-N bond length of the oxidized state of [CuI(dppS)2]+ after electron injection to TiO2 NPs shortens by 0.05 Å compared to that in the ground state. The interpretation of these observed structural changes associated with excited and charge separated states will be discussed. These results not only set an example for applying XTA in capturing the intermediate structure of metal complex/semiconductor NP hybrids but also provide guidance for designing efficient CuI diimine complexes with optimized structures for application in solar-to-electricity conversion. This journal is
Automated Micro Hall Effect measurements
With increasing complexity of processes and variety of materials used for semiconductor devices, stringent control of the electronic properties is becoming ever more relevant. Collinear micro four-point probe (M4PP) based measurement systems have become high-end metrology methods for characterization and monitoring of sheet resistance as well as sheet carrier density and mobility via the Micro Hall Effect (MHE) method.

General information
State: Published
Organisations: Department of Micro- and Nanotechnology, Nanointegration, Department of Physics, Experimental Surface and Nanomaterials Physics, Silicon Microtechnology, Capres A/S
Authors: Petersen, D. H. (Intern), Henrichsen, H. H. (Intern), Lin, R. (Ekstern), Nielsen, P. F. (Ekstern), Hansen, O. (Intern)
Number of pages: 2
Pages: 37-38
Publication date: 2014

Host publication information
Title of host publication: Proceedings of the 2014 7th International Silicon-Germanium Technology and Device Meeting
Main Research Area: Technical/natural sciences
Conference: 2014 7th International Silicon-Germanium Technology and Device Meeting, Singapore, Singapore, 02/06/2014 - 02/06/2014
DOIs: 10.1109/ISTDM.2014.6874677
Source: FindIt
Source-ID: 269972295
Publication: Research - peer-review » Conference abstract in proceedings – Annual report year: 2014

Axion helioscopes update: the status of CAST & IAXO
Almost 35 years since their suggestion as a good solution to the strong CP-problem, axions remain one of the few viable candidates for the Dark Matter, although still eluding detection. Most of the methods for their detection are based on their coupling to photons, one of the most sensitive ones being the helioscope technique. We report on the current status of the
CERN Axion Solar Telescope and the future International Axion Observatory (IAXO). Recent results from the second part of CAST phase II, where the magnet bores were filled with $^3$He gas at variable pressure achieving sensibilities on the axion mass up to 1.2 eV, are presented. Currently, CAST is expecting to improve its sensitivity to solar axions with rest mass below 0.02 eV/c$^2$ after the upgrade of the X-ray detectors and with the implementation of a second X-ray optic. At the same time, it is exploring other possibilities at the low energy physics frontier. On the other hand, IAXO, the fourth generation axion helioscope, aims to improve CAST’s performance in terms of axionphoton coupling by 1-1.5 orders of magnitude. The details of the project building a dedicated magnet, optics and X-ray detectors are given.

**Bandgap calculations and trends of organometal halide perovskites**

Energy production from the Sun requires a stable efficient light absorber. Promising candidates in this respect are organometal perovskites (ABX$_3$), which have been intensely investigated during the last years. Here, we have performed electronic structure calculations of 240 perovskites composed of Cs, CH$_3$NH$_3$, and HC(NH$_2$)$_2$ as A-cation, Sn and Pb as B-ion, and a combination of Cl, Br, and I as anions. The calculated gaps span over a region from 0.5 to 5.0 eV. In addition, the trends over bandgaps have been investigated: the bandgap increases with an increase of the electronegativities of the constituent species, while it reduces with an increase of the lattice constants of the system.
Bathtub physics

General information
State: Published
Organisations: Department of Physics, Biophysics and Fluids
Authors: Andersen, A. P. (Intern)
Number of pages: 1
Pages: 88-88
Publication date: 2014
Main Research Area: Technical/natural sciences

Publication information
Journal: Physics Today
Volume: 67
Issue number: 10
ISSN (Print): 0031-9228
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Scopus rating (2017): SNIP 1.129 SJR 0.66 CiteScore 1.14
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): SJR 0.726 SNIP 1.172 CiteScore 1.38
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.733 SNIP 1.6 CiteScore 1.39
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.024 SNIP 1.902 CiteScore 1.64
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.277 SNIP 1.717 CiteScore 1.99
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.631 SNIP 1.789 CiteScore 1.84
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.599 SNIP 1.703 CiteScore 1.46
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 0.918 SNIP 1.499
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 0.749 SNIP 1.206
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.991 SNIP 1.73
Scopus rating (2007): SJR 1.192 SNIP 2.362
Scopus rating (2006): SJR 1.303 SNIP 2.385
Scopus rating (2005): SJR 1.333 SNIP 3.23
Scopus rating (2004): SJR 1.148 SNIP 3.373
Scopus rating (2003): SJR 1.084 SNIP 3.004
Scopus rating (2002): SJR 2.51 SNIP 2.803
Benchmarking the Stability of Oxygen Evolution Reaction Catalysts: The Importance of Monitoring Mass Losses

Because of the rising need for energy storage, potentially facilitated by electrolyzers, improvements to the catalysis of the oxygen evolution reaction (OER) become increasingly relevant. Standardized protocols have been developed for determining critical figures of merit, such as the electrochemical surface area, mass activity and specific activity. Even so, when new and more active catalysts are reported, the catalyst stability tends to play a minor role. In this work, we monitor corrosion on RuO$_2$ and MnO$_x$ by combining the electrochemical quartz crystal microbalance (EQCM) with inductively coupled plasma mass spectrometry (ICP–MS). We show that a meaningful estimation of the stability cannot be achieved based on purely electrochemical tests. On the catalysts tested, the anodic dissolution current was four orders of magnitude lower than the total current. We propose that even if long-term testing cannot be replaced, a useful evaluation of the stability can be achieved with short-term tests by using EQCM or ICP–MS.

Beyond the volcano limitations in electrocatalysis - oxygen evolution reaction

Oxygen evolution catalysis is restricted by the interdependence of adsorption energies of the reaction intermediates and the surface reactivity. The interdependence reduces the number of degrees of freedom available for catalyst optimization. Here it is demonstrated that this limitation can be removed by active site modification. This can be achieved on ruthenia by...
incorporation of Ni or Co into the surface, which activates a proton donor-acceptor functionality on the conventionally inactive bridge surface sites. This enhances the actual measured oxygen evolution activity of the catalyst significantly compared to conventional ruthenia.
Bifurcation Analysis and Dimension Reduction of a Predator-Prey Model for the L-H Transition

General information
State: Published
Organisations: Department of Applied Mathematics and Computer Science, Mathematics, Department of Physics, Plasma Physics and Fusion Energy, Chinese Academy of Sciences
Authors: Dam, M. (Intern), Brøns, M. (Intern), Juul Rasmussen, J. (Intern), Naulin, V. (Intern), Xu, G. (Eksterm)
Number of pages: 1
Publication date: 2014
Event: Poster session presented at 51st Culham Plasma Physics Summer School, Abingdon, Oxfordshire, United Kingdom.
Main Research Area: Technical/natural sciences
Electronic versions:
LH_transition_poster_Magnus.pdf

Blueshift of the silver plasmon band using controlled nanoparticle dissolution in aqueous solution

In this work, we report the size-dependent blue shift of the silver nanoparticle plasmon band in aqueous solution by means of UV/Vis spectroscopy. An oxidative dissolution scheme allows a gradual decrease in the particle sizes by controlled oxidation during recording of the optical spectra. Hence, all sizes until complete dissolution can be obtained on the same substrate, thereby avoiding substrate-to-substrate variations and greatly increasing the size resolution. Cyanide and cysteamine are strong nucleophiles (electron pair donors) that deposits negative charge onto the NP surface. A 1/R-dependence of the plasmon peak energy is seen, which is interpreted as an increase in the free electron density of the nanoparticles.

Utilization of the size-dependent electronic contribution to the optical response in nanoplasmonic sensors is shown to be a promising extension to improve the sensitivity and specificity, as compared to traditional refractive index sensing.

General information
State: Published
Bromosubstituted norbornadienes and their reversible photolytic transformation to quadricyclanes

Two new model systems for use within the rapidly developing ultrafast time resolved x-ray scattering techniques have been prepared. Their photoisomerisation from norbornadiene to quadricyclane was found to be a suitable reaction to follow. Simulations of scattering patterns (not included in this report) showed that if heavy atoms are included in these molecular structures, then the transformation can be followed by transient x-ray scattering techniques. Two new bromosubstituted norbornadienes were synthesised and characterised. Absorption spectroscopy showed that the norbornadienes are converted quantitatively to quadricyclanes under UV irradiation. NMR studies showed that the process was fully reversible and that the norbornadienes could be completely recovered even without addition of catalysts. Furthermore, it was shown that the formation of quadricyclane from norbornadiene was unaffected by triplet sensitizers. The two new model systems synthesised thus are strong candidates for use in time resolved x-ray scattering studies both in gas and condensed phases.

Calculated Pourbaix Diagrams of Cubic Perovskites for Water Splitting: Stability Against Corrosion

We use density functional theory calculations to investigate the stability of cubic perovskites for photo-electrochemical water splitting taking both materials in their bulk crystal structure and dissolved phases into account. The method is validated through a detailed comparison of the calculated and experimental Pourbaix diagrams for TiO2 and ZnO. For a class of 23 oxides, oxynitrides, and oxyfluorides, which were recently proposed as candidates for one-photon water splitting, our calculations predict most of the materials to be stable at potentials around the water red-ox level. The oxides become less stable at lower potentials, while the oxynitrides become unstable at higher potentials. We discuss the implications of these findings for the problem of photo-corrosion of water splitting electrodes.
CAMEA ESS: The Continuous Angle Multi-Energy Analysis Indirect Geometry Spectrometer for the European Spallation Source

The CAMEA ESS neutron spectrometer is designed to achieve a high detection efficiency in the horizontal scattering plane, and to maximize the use of the long pulse European Spallation Source. It is an indirect geometry time-of-flight spectrometer that uses crystal analysers to determine the final energy of neutrons scattered from the sample. Unlike other indirect geometry spectrometers CAMEA will use ten concentric arcs of analysers to analyse scattered neutrons at ten different final energies, which can be increased to 30 final energies by use of prismatic analysis. In this report we will outline the CAMEA instrument concept, the large performance gain, and the potential scientific advancements that can be made with this instrument.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Ecole Polytechnique Federale de Lausanne (EPFL), University of Copenhagen, Paul Scherrer Institut
Authors: Freeman, P. (Ekstern), Birk, J. (Ekstern), Marko, M. (Ekstern), Bertelsen, M. (Ekstern), Larsen, J. (Intern), Christensen, N. B. (Intern), Lefmann, K. (Ekstern), Jacobsen, J. (Ekstern), Niedermayer, C. (Ekstern), Juranyi, F. (Ekstern), Ronnow, H. (Ekstern)
Number of pages: 7
Pages: 03005
Publication date: 2014
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Physics: Conference Series (Online)
Volume: 83
ISSN (Print): 1742-6596
Ratings:
BFI (2018): BFI-level 1
BFI (2017): BFI-level 1
Scopus rating (2017): CiteScore 0.48 SJR 0.241 SNIP 0.447
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 0.45 SJR 0.24 SNIP 0.401
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.252 SNIP 0.374 CiteScore 0.35
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.264 SNIP 0.352 CiteScore 0.32
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.245 SNIP 0.293 CiteScore 0.25
ISI indexed (2013): ISI indexed no
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Catalysts for selective oxidation of ammonia in a gas containing hydrogen

The invention contributes to a cost effective way to solve the problem of trace ammonia removal from hydrogen containing gas. The set of catalysts of the invention selectively oxidised ammonia in ppm concentration even in gas mixture containing hydrogen gas in concentration of three orders of magnitude higher than the concentration of ammonia.

General information
State: Published
Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics
Authors: Chakraborty, D. (Intern), Olesen, S. E. (Intern), Chorkendorff, I. (Intern)
Publication date: 2014
Chemical preparation and spectroscopic characterization of plasmonic silver nanoparticles using fruits as reducing agent.

General information
State: Published
Organisations: Department of Physics, Biophysics and Fluids, Department of Micro- and Nanotechnology, Fluidic Array Systems and Technology, Technical University of Denmark
Authors: Hyllested, J. (Ekstern), Espina Palanco, M. (Intern), Hagen, N. (Ekstern), Mogensen, K. B. (Intern), Kneipp, K. (Intern)
Number of pages: 2
Publication date: 2014

Projects:
Design of magnetic nanoparticle-materials for induction heating
Department of Physics
Period: 01/06/2018 → 31/05/2021
Number of participants: 4
Phd Student: Langemark, Nikolaj Ørbæk (Intern)
Supervisor: Chorkendorff, Ib (Intern)
Damsgaard, Christian Danvad (Intern)
Main Supervisor: Frandsen, Cathrine (Intern)
Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Exploring new catalysts for conversion of sustainable energy by testing activity of mass-selected atoms, clusters and nanoparticles
Department of Physics
Period: 01/06/2018 → 31/05/2021
Number of participants: 3
Phd Student: Krabbe, Alexander (Intern)
Supervisor: Kibsgaard, Jakob (Intern)
Main Supervisor: Chorkendorff, Ib (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Samfinansierede - Virksomhed
Project: PhD

**Atomic-scale computational modeling of light-matter interactions in materials for opto-electronic applications**

Department of Physics
Period: 15/05/2018 → 14/05/2021
Number of participants: 3
Phd Student: Manti, Simone (Intern)
Supervisor: Hansen, Ole (Intern)
Main Supervisor: Thygesen, Kristian Sommer (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Anden EU-finansiering
Project: PhD

**From Single Atoms to Clusters: Measuring Catalytic Activity for Energy Conversion**

Department of Physics
Period: 01/04/2018 → 31/03/2021
Number of participants: 3
Phd Student: Hansen, Johannes Novak (Intern)
Supervisor: Kibsgaard, Jakob (Intern)
Main Supervisor: Chorkendorff, Ib (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet
Project: PhD

**Generation of macroscopic states of light for quantum sensing and information processing**

Department of Physics
Period: 01/04/2018 → 31/03/2021
Number of participants: 4
Phd Student: Arnbak, Jens (Ekstern)
Supervisor: Gehring, Tobias (Intern)
Neergaard-Nielsen, Jonas Schou (Intern)
Main Supervisor: Andersen, Ulrik Lund (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Grundforskningsfonden
Project: PhD
Generation of macroscopic states of light for quantum sensing and information processing
Department of Physics
Period: 01/04/2018 → 31/03/2021
Number of participants: 4
Phd Student:
Ambak, Jens (Intern)
Supervisor:
Gehring, Tobias (Intern)
Neergaard-Nielsen, Jonas Schou (Intern)
Main Supervisor:
Andersen, Ulrik Lund (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Grundforskningsfonden
Project: PhD

Investigation of wide-bandgap photoabsorber for tandem devices
Department of Physics
Period: 01/04/2018 → 31/03/2021
Number of participants: 3
Phd Student:
Youngman, Tomas Hugh (Intern)
Supervisor:
Chorkendorff, Ib (Intern)
Main Supervisor:
Vesborg, Peter Christian Kjærgaard (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet
Project: PhD

Crystallization Fundamentals of Polymers and Oligomers
Department of Physics
Period: 01/03/2018 → 28/02/2021
Number of participants: 3
Phd Student:
Huss-Hansen, Mathias Kasper (Intern)
Supervisor:
Balzano, Luigi (Ekstern)
Main Supervisor:
Knaapila, Matti (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansierede - Virksomhed
Project: PhD

Dosimetry for low energy x-rays
Department of Physics
Period: 01/12/2017 → 30/11/2020
Number of participants: 4
Phd Student:
Hjørringgaard, Jakob Grünewald (Intern)
Supervisor:
Ankjærgaard, Christina (Intern)
Miller, Arne (Intern)
Main Supervisor:
Lindvold, Lars René (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Nanoscale Characterisation of Metal Films Adhesion for Plasmonic Applications
Department of Physics
Period: 01/12/2017 → 30/11/2020
Number of participants: 4
Phd Student:
Heinig, Mario (Intern)
Supervisor:
Jansen, Henri (Intern)
Wagner, Jakob Birkedal (Intern)
Main Supervisor:
Kadkhodazadeh, Shima (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Neutronics and thermal hydraulics simulations of multi-fluid nuclear reactors
Department of Physics
Period: 01/12/2017 → 30/11/2020
Number of participants: 3
Phd Student:
Nalbandyan, Ashkhen (Intern)
Supervisor:
Lauritzen, Bent (Intern)
Main Supervisor:
Klinkby, Esben Bryndt (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Smoothed advanced silicon NEMS devices
Department of Physics
Period: 01/12/2017 → 30/11/2020
Number of participants: 4
Phd Student:
Nguyen, Vy Thi Hoang (Intern)
Supervisor:
Hübner, Jörg (Intern)
Jensen, Flemming (Intern)
Main Supervisor:
Jansen, Henri (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD
Development of ultra-high quality mechanical oscillators

Department of Physics
Period: 01/11/2017 → 31/10/2020
Number of participants: 3
Phd Student: Høj, Dennis (Intern)
Supervisor: Sigmund, Ole (Intern)
Main Supervisor: Andersen, Ulrik Lund (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Grundforskningsfonden
Project: PhD

Multiscale coarsening studied by Dark Fields X-ray Microscopy

Department of Physics
Period: 01/11/2017 → 31/10/2020
Number of participants: 2
Phd Student: Kutsal, Mustafacan (Intern)
Main Supervisor: Poulsen, Henning Friis (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Ansat eksternt
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

Non-Gaussian Cluster States

Department of Physics
Period: 01/10/2017 → 30/09/2020
Number of participants: 3
Phd Student:
Larsen, Mikkel Vilsbøll (Intern)
Supervisor:
Neergaard-Nielsen, Jonas Schou (Intern)
Main Supervisor:
Andersen, Ulrik Lund (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Error Reconciliation Protocols for Continuous-Variable Quantum Key Distribution
Department of Physics
Period: 01/09/2017 → 31/08/2020
Number of participants: 4
Phd Student:
Mani, Hossein (Intern)
Supervisor:
Gehring, Tobias (Intern)
Pacher, Christoph (Ekstern)
Main Supervisor:
Andersen, Ulrik Lund (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Fonde
Project: PhD

Comparison of Tokamak Plasma Midplane with Divertor Conditions and Consequences for Modelling
Department of Physics
Period: 01/08/2017 → 31/07/2020
Number of participants: 3
Phd Student:
Nem, Raheesty Devi (Ekstern)
Supervisor:
Eich, Thomas Hubert (Ekstern)
Main Supervisor:
Naulin, Volker (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Comparison of Tokamak Plasma Midplane with Divertor Conditions and Consequences for Modelling
Department of Physics
Period: 01/08/2017 → 31/07/2020
Number of participants: 3
Phd Student:
Nem, Raheesty Devi (Intern)
Supervisor:
Eich, Thomas Hubert (Ekstern)
Main Supervisor:
Naulin, Volker (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD
Electrolysis of Water: New Catalyst for the Oxygen Evolution Reaction

Department of Physics
Period: 01/08/2017 → 31/07/2020
Number of participants: 4
Phd Student:
Moon, Choongman (Ekstern)
Supervisor:
Kibsgaard, Jakob (Intern)
Stephens, Ifan (Intern)
Main Supervisor:
Chorkendorff, Ib (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet
Project: PhD

Electrolysis of Water: New Catalyst for the Oxygen Evolution Reaction

Department of Physics
Period: 01/08/2017 → 31/07/2020
Number of participants: 4
Phd Student:
Moon, Choongman (Intern)
Supervisor:
Kibsgaard, Jakob (Intern)
Stephens, Ifan (Intern)
Main Supervisor:
Chorkendorff, Ib (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet
Project: PhD

Theoretical studies of materials for water splitting

Department of Physics
Period: 01/08/2017 → 31/07/2020
Number of participants: 3
Phd Student:
Garijo del Río, Estefanía (Intern)
Supervisor:
Thygesen, Kristian Sommer (Intern)
Main Supervisor:
Jacobsen, Karsten Wedel (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet
Project: PhD

Computational studies of two-dimension materials and heterosstructures

Department of Physics
Period: 15/07/2017 → 14/07/2020
Number of participants: 3
Phd Student:
Riis-Jensen, Anders Christian (Intern)
Supervisor:
Jacobsen, Karsten Wedel (Intern)
Main Supervisor:
Thygesen, Kristian Sommer (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

**Velocity-space tomography from KeV MeV-range ions in fusion plasmas**
Department of Physics
Period: 01/07/2017 → 30/06/2020
Number of participants: 3
Phd Student:
Madsen, Birgitte (Intern)
Supervisor:
Huang, Juan (Ekstern)
Main Supervisor:
Salewski, Mirko (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Anden EU-finansiering
Project: PhD

**Multi-Scale 3D Imaging of Heterogeneous Nucleation in Ferroelectrics**
Department of Physics
Period: 15/06/2017 → 14/06/2020
Number of participants: 4
Phd Student:
Ormstrup, Jeppe (Intern)
Supervisor:
Matheiesen, Ragnvald (Ekstern)
Simons, Hugh (Intern)
Main Supervisor:
Poulsen, Henning Friis (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

**Electrochemical N2 reduction under ambient conditions**
Department of Physics
Period: 01/04/2017 → 31/03/2020
Number of participants: 5
Phd Student:
Andersen, Suzanne Zamany (Intern)
Supervisor:
Chorkendorff, Ib (Intern)
Kibsgaard, Jakob (Intern)
Vesborg, Peter Christian Kjærgaard (Intern)
Main Supervisor:
Vesborg, Peter Christian Kjærgaard (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet
Project: PhD

Quantum Communication with non-Gaussian states
Department of Physics
Period: 01/04/2017 → 31/03/2020
Number of participants: 3
Phd Student:
Breum, Casper Rubæk (Intern)
Supervisor:
Neergaard-Nielsen, Jonas Schou (Intern)
Main Supervisor:
Andersen, Ulrik Lund (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Simulation of Three-Wave Interactions in Microwave Heated Fusion Plasmas
Department of Physics
Period: 01/04/2017 → 31/03/2020
Number of participants: 4
Phd Student:
Senstius, Mads Givskov (Intern)
Supervisor:
Madsen, Jens (Intern)
Vann, Roddy (Ekstern)
Main Supervisor:
Nielsen, Stefan Kragh (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Fonde
Project: PhD

2-Dimensional Materials as Substrate and base materials for catalytic reactive centers
Department of Physics
Period: 15/03/2017 → 14/03/2020
Number of participants: 3
Phd Student:
Secher, Niklas Mørch (Intern)
Supervisor:
Kibsgaard, Jakob (Intern)
Main Supervisor:
Chorkendorff, Ib (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Induction-heated catalytic hydrogen production - amagnetic investigation
Department of Physics
Period: 15/03/2017 → 14/03/2020
Number of participants: 3
Phd Student:
Almind, Mads Radmer (Intern)
The Correlation of Reactivity and Activity of Mass Selected Nanoparticles

Department of Physics
Period: 15/03/2017 → 14/03/2020
Number of participants: 3
Phd Student:
Sørensen, Jakob Ejler (Intern)
Supervisor:
Kibsgaard, Jakob (Intern)
Main Supervisor:
Chorkendorff, Ib (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet
Project: PhD

Theory and modeling of acoustic streaming in microfluidic devices

Department of Physics
Period: 01/03/2017 → 29/02/2020
Number of participants: 3
Phd Student:
Bach, Jacob Søberg (Intern)
Supervisor:
Bohr, Tomas (Intern)
Main Supervisor:
Bruus, Henrik (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Quantum-optical networks with solid state spins and photons

Department of Physics
Period: 01/02/2017 → 30/04/2017
Number of participants: 3
Phd Student:
Yakovlev, George (Intern)
Supervisor:
Huck, Alexander (Intern)
Main Supervisor:
Andersen, Ulrik Lund (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD
Chiral Magnetism from Mean Field Theory

Department of Physics
Period: 01/01/2017 → 31/12/2019
Number of participants: 4
Phd Student:
Torelli, Daniele (Intern)
Supervisor:
Christensen, Niels Bech (Intern)
Olsen, Thomas (Intern)
Main Supervisor:
Jacobsen, Karsten Wedel (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Investigations on deep UV and NIR transitions in feldspars for novel applications in luminescence dosimetry

Department of Physics
Period: 15/12/2016 → 14/12/2019
Number of participants: 3
Phd Student:
Kumar, Raju (Intern)
Supervisor:
Kook, Myung Ho (Intern)
Main Supervisor:
Jain, Mayank (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Fabrication and Magnetic characterization of layered structures by means of election holography

Department of Physics
Period: 01/12/2016 → 30/11/2019
Number of participants: 4
Phd Student:
Hyllested, Jes Ærøe (Intern)
Supervisor:
Jensen, Flemming (Intern)
Wagner, Jakob Birkedal (Intern)
Main Supervisor:
Kasama, Takeshi (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Neutrals in the East Sol/Edge region and their impact on plasma operation

Department of Physics
Period: 15/11/2016 → 24/01/2020
Number of participants: 3
Phd Student:
Sindbjerg Poulsen, Aslak (Intern)
Supervisor:
Li, Jiangang (Ekstern)
Main Supervisor:
Naulin, Volker (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet
Project: PhD

4D Seismics for Fracture Characterization
Department of Physics
Period: 15/10/2016 → 14/10/2019
Number of participants: 2
Phd Student:
Sören Dramsch, Jesper (Intern)
Main Supervisor:
Lüthje, Mikael (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Investigations of high speed neutral particle injection into K-STAR plasmas
Department of Physics
Period: 15/10/2016 → 14/10/2019
Number of participants: 3
Phd Student:
Avdeeva, Galina (Ekstern)
Supervisor:
Choe, Wonho (Ekstern)
Main Supervisor:
Naulin, Volker (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Investigations of high speed neutral particle injection into K-STAR plasmas
Department of Physics
Period: 15/10/2016 → 14/10/2019
Number of participants: 3
Phd Student:
Avdeeva, Galina (Intern)
Supervisor:
Choe, Wonho (Ekstern)
Main Supervisor:
Naulin, Volker (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
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 Behrensdorff (Intern)

Implementation of fiber-based continuous-variable quantum key distribution protocols

Department of Physics
Period: 01/10/2016 → 30/09/2019
Number of participants: 3
Phd Student:
Solar Nikolic, Dino (Intern)
Supervisor:
Gehring, Tobias (Intern)
Main Supervisor:
Andersen, Ulrik Lund (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Offentlig finansiering
Project: PhD

CO2 reduction on model catalyst surfaces

Department of Physics
Period: 01/09/2016 → 31/08/2019
Number of participants: 4
Phd Student:
Vagn Hogg, Thomas (Intern)
Supervisor:
Seger, Brian (Intern)
Elucidating the mechanistic pathways of carbon dioxide electroreduction

Department of Physics
Period: 01/09/2016 → 31/08/2019
Number of participants: 4
Phd Student:
Scott, Søren Bertelsen (Intern)
Supervisor:
Rossmeisl, Jan (Intern)
Stephens, Ifan (Intern)
Main Supervisor:
Chorkendorff, Ib (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansierede - Virksomhed
Project: PhD

Induction-Heated Hydrogen Production

Department of Physics
Period: 01/09/2016 → 31/08/2019
Number of participants: 4
Phd Student:
Wismann, Sebastian Thor (Intern)
Supervisor:
Frandsen, Cathrine (Intern)
Mortensen, Peter Mølgaard (Intern)
Main Supervisor:
Chorkendorff, Ib (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

In situ Electron Microscopy Characterization of Catalysts for Sustainable Energy

Department of Physics
Period: 01/09/2016 → 31/08/2019
Number of participants: 4
Phd Student:
Nielsen, Monia Runge (Intern)
Supervisor:
08052011, Emma (Ekstern)
Wagner, Jakob Birkedal (Intern)
Main Supervisor:
Hansen, Thomas Willum (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet
Project: PhD
Model-optimized Screening of Checked-in Luggage

Department of Physics
Period: 01/09/2016 → 31/08/2019
Number of participants: 5
Phd Student:
Busi, Matteo (Intern)
Supervisor:
Frisvad, Jeppe Revall (Intern)
Bergbäck Knudsen, Erik (Intern)
Olsen, Ulrik Lund (Intern)
Main Supervisor:
Haldrup, Kristoffer (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Offentlig finansiering
Project: PhD

On Parametric Decay of Electron Cyclotron Heating Beams in ASDEX Upgrade

Department of Physics
Period: 01/09/2016 → 31/08/2019
Number of participants: 4
Phd Student:
Hansen, Søren Kjer (Ekstern)
Supervisor:
Pedersen, Morten Stejner (Intern)
Stober, Jörg Karl (Ekstern)
Main Supervisor:
Nielsen, Stefan Kragh (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Ansat eksternt
Project: PhD

The catalysis of the selective electrochemical oxidation of hydrocarbons

Department of Physics
Period: 01/09/2016 → 31/08/2019
Number of participants: 3
Phd Student:
Winiwarter, Anna (Intern)
Supervisor:
Seger, Brian (Intern)
Main Supervisor:
Chorkendorff, Ib (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Offentlig finansiering
Project: PhD

Ultrafast electronic and coupled electronic-nuclear dynamics of solvated metal complexes

Department of Physics
Period: 01/09/2016 → 31/08/2019
Number of participants: 4
Phd Student:
Electrodeposition of Metallic 3D Surface-Profles 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-lamentary 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 surfacepro les 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 eect during subsequent physical vapor deposition (PVD) of layers, thereby creating self-formed and physically separated superconductor laments 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 lamentization 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.
Fiber-coupled scintillator dosimetry for proton therapy
Department of Physics
Period: 15/08/2016 → 14/08/2019
Number of participants: 3
Phd Student:
Christensen, Jeppe Brage (Intern)
Supervisor:
Grau, Cai (Ekstern)
Main Supervisor:
Andersen, Claus E. (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet
Project: PhD

Generation of Macroscopic Squeezed States for Quantum Sensing
Department of Physics
Period: 01/08/2016 → 30/11/2017
Number of participants: 3
Phd Student:
Pedersen, Mikkel Maag (Intern)
Supervisor:
Gehring, Tobias (Intern)
Main Supervisor:
Andersen, Ulrik Lund (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

On-Chip quantum communication
Department of Physics
Period: 01/08/2016 → 31/07/2019
Number of participants: 3
Phd Student:
Kordts, Arne (Ekstern)
Supervisor:
Gehring, Tobias (Intern)
Main Supervisor:
Andersen, Ulrik Lund (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Offentlig finansiering
Project: PhD
Main Supervisor:
Andersen, Ulrik Lund (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Offentlig finansiering
Project: PhD

System-level simulation and automation of microscale acoustofluidics for biotechnology
Department of Physics
Period: 15/06/2016 → 14/06/2019
Number of participants: 4
Phd Student:
Skov, Nils Refstrup (Intern)
Supervisor:
Stokke, Bjørn Torger (Ekstern)
Wiklund, Martin (Ekstern)
Main Supervisor:
Bruus, Henrik (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

A target diagnostic imaging system for ESS
Department of Physics
Period: 01/06/2016 → 31/05/2019
Number of participants: 3
Phd Student:
Borghi, Nicolo (Intern)
Supervisor:
Zanini, Luca (Ekstern)
Main Supervisor:
Lauritzen, Bent (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansierede - Virksomhed
Project: PhD

Atomic-scale modelling of interfaces in electronic devices
Department of Physics
Period: 01/06/2016 → 03/02/2021
Number of participants: 5
Phd Student:
Jelver, Line (Intern)
Supervisor:
Stokbro, Kurt (Intern)
Stradi, Daniele (Intern)
Thygesen, Kristian Sommer (Intern)
Main Supervisor:
Jacobsen, Karsten Wedel (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Industrial PhD
Project: PhD
Electron microscopy of noble metal catalysts for automotive exhaust abatement
Department of Physics
Period: 01/06/2016 → 31/05/2019
Number of participants: 3
Phd Student:
Jespersen, Sebastian Pirel Fredsgaard (Intern)
Supervisor:
Helveg, Stig (Ekstern)
Main Supervisor:
Damsgaard, Christian Danvad (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansierede - Virksomhed
Project: PhD

Fundamental investigations of electrocatalytic H2O2 production
Department of Physics
Period: 01/05/2016 → 01/07/2016
Number of participants: 3
Phd Student:
Ebert, Kenneth (Intern)
Supervisor:
Chorkendorff, Ib (Intern)
Main Supervisor:
Stephens, Ifan (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Offentlig finansiering
Project: PhD

Cavity-modified dynamics of Nitrogen-Vacancy centers in Diamond
Department of Physics
Period: 15/02/2016 → 14/03/2019
Number of participants: 3
Phd Student:
Jensen, Rasmus (Intern)
Supervisor:
Huck, Alexander (Intern)
Main Supervisor:
Andersen, Ulrik Lund (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

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)

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 Gd_{0.1}Ce_{0.9}O_{1.95-δ}La_{0.6}Sr_{0.4}FeO_{3-δ}-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-Al_{2}O_{3} egg-shell catalyst for H_2 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:
Improving the decision base for emergency management in the event of airborne radioactive contamination of city areas

Wulff, Anders Christian (Intern)
Phd Student:
Hinrichsen, Yvonne (Intern)
Supervisor:
Roos, Per (Intern)
Main Supervisor:
Andersson, Kasper Grann (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)

Phase-Contrast Imaging of Plasma Density Fluctuations in Wendelstein 7-X

Böttger, Lukas-Georg (Intern)
Supervisor:
Gruke, Olaf (Ekstern)
Main Supervisor:
Naulin, Volker (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Ansat eksternt

Squeezed-light enhanced quantum opto-mechanics

Bilek, Jan (Intern)
Main Supervisor:
Andersen, Ulrik Lund (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)

Development of new Electrocatalysts for Low or Intermediate Temperature Fuel Cells and Electrolyzers

Maagaard, Thomas (Intern)
Supervisor:
Horch, Sebastian (Intern)
Main Supervisor:
Chorkendorff, Ib (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Small-field dosimetry standard for MV photon beams
Department of Physics
Period: 01/12/2015 → 30/11/2018
Number of participants: 3
Phd Student:
Santurio, Grichar Valdes (Intern)
Supervisor:
Helt-Hansen, Jakob (Intern)
Main Supervisor:
Andersen, Claus E. (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Experimental solid state Nano-Optics
Department of Physics
Period: 01/11/2015 → 31/10/2018
Number of participants: 3
Phd Student:
Boll, Mads Kjær (Intern)
Supervisor:
Huck, Alexander (Intern)
Main Supervisor:
Andersen, Ulrik Lund (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Technology Development for Sillicon NEMS devices
Department of Physics
Period: 01/11/2015 → 31/10/2018
Number of participants: 4
Phd Student:
Chang, Bingdong (Intern)
Supervisor:
Hübner, Jörg (Intern)
Jansen, Henri V. (Ekstern)
Main Supervisor:
Jensen, Flemming (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD
Atomic-scale modelling of carrier dynamics in photo-excited semi-conductors

Department of Physics
Period: 01/10/2015 → 30/09/2018
Number of participants: 3
Phd Student:
Haastrup, Sten (Intern)
Supervisor:
Jacobsen, Karsten Wedel (Intern)
Main Supervisor:
Thygesen, Kristian Sommer (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Investigating the role of charge imbalance on the luminescence response of quartz and feldspars

Department of Physics
Period: 01/10/2015 → 30/09/2018
Number of participants: 3
Phd Student:
Autzen, Martin (Intern)
Supervisor:
Jain, Mayank (Intern)
Main Supervisor:
Buylaert, Jan-Pieter (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Anden EU-finansiering
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)
Project
Cost and energy effective all-black solar cell panel | Black Si BIPV | Phase 1
The project will aim at establish a method for proof-of-concept creation of working modules with black silicon cells and black front grid. A few prototype modules of medium quality will be fabricated and be used for probing the market interest for the all black silicon technology, and further verify the superior angular light absorption on the module level. The projects falls into the following work packages:

•Investigation of interconnection method
•Investigation/proof-of-concept of black electroplating methods to make the silver front fingers black
•Design and production of Black Silicon cells with black fingers
•Investigation of module technology supporting the all black silicon cell, proof-of-concept production and module characterization.
•Proof-of-Business of Black Silicon BIPV

The project is a major step in making the black silicon technology available to the Danish PV industry being strong in BIPV where the technology is very well suited.

Department of Photonics Engineering
Diode Lasers and LED Systems
Department of Micro- and Nanotechnology
Silicon Microtechnology
Experimental Surface and Nanomaterials Physics
Period: 01/07/2015 → 01/10/2016
Number of participants: 4
Acronym: Black-Si-BIPV
Project participant:
Thorsteinsson, Sune (Intern)
Davidsen, Rasmus Schmidt (Intern)
Hansen, Ole (Intern)
Project Manager, academic:
Poulsen, Peter Behrensdorff (Intern)

Studies of Coherent Structures in Magnetically Confined Plasmas
Department of Physics
Period: 01/07/2015 → 30/06/2018
Number of participants: 4
Phd Student:
Olsen, Jeppe Miki Busk (Intern)
Supervisor:
Madsen, Jens (Intern)
Nielsen, Anders Henry (Intern)
Main Supervisor:
Rasmussen, Jens Juul (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet
Project: PhD

Synthesis and characterisation of active and active Pt alloys catalysts for oxygen electroreduction
Department of Physics
Period: 01/06/2015 → 31/05/2018
Number of participants: 7
Phd Student:
Roy, Claudie (Intern)
Supervisor:
Kibsgaard, Jakob (Intern)
Efficient, two-photon water splitting photoelectrode

Department of Physics
Period: 01/03/2015 → 13/06/2018
Number of participants: 6
Phd Student:
Bækbo, Martin Jesper (Intern)
Supervisor:
Chorkendorff, Ib (Intern)
Main Supervisor:
Vesborg, Peter Christian Kjærgaard (Intern)
Examiner:
Seger, Brian (Intern)
Bandarenka, Aliaksandr (Intern)
Georg Jaegermann, Wolfram (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Offentlig finansiering
Project: PhD

Improving Quality of Motion Managed Radiotherapy for Lung Cancer Patients

Department of Physics
Period: 01/03/2015 → 06/06/2018
Number of participants: 6
Phd Student:
Sibolt, Patrik (Intern)
Supervisor:
Behrens, Claus F. (Ekstern)
Main Supervisor:
Andersen, Claus E. (Intern)
Examiner:
Lauritzen, Bent (Intern)
Poulsen, Per Rugaard (Ekstern)
Seco, Joao (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Computational study of sel-formation in Li-ion batteries

Department of Physics
Period: 15/02/2015 → 31/05/2015
Number of participants: 2
Phd Student:
Financing sources
Source: Internal funding (public)
Name of research programme: Eksternt finansieret virksomhed
Project: PhD

**Ecoli Morphology Analysis**

13 week

Center for Electron Nanoscopy

DTU Danchip

Department of Physics

Experimental Surface and Nanomaterials Physics

Period: 11/02/2015 → 18/05/2015

Number of participants: 4

Project participant:
Lyngby Bregendahl, Anders (Ekstern)
Schultz Carstensen, Marcus (Ekstern)

Supervisor:
Damsgaard, Christian Danvad (Intern)

Main Supervisor:
Mateiu, Ramona Valentina (Intern)

**CO2 electroreduction on nanostructured catalysts**

Department of Physics

Period: 01/02/2015 → 16/05/2018

Number of participants: 6

Phd Student:
Bertheussen, Erlend (Intern)

Supervisor:
Stephens, Ifan (Intern)

Main Supervisor:
Chorkendorff, Ib (Intern)

Examiner:
Damsgaard, Christian Danvad (Intern)
Ill, Joel W. Ager (Ekstern)
Rodriguez, Paramaconi (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

**Computer Simulation of the 3D structure of Materials**

Department of Physics

Period: 01/02/2015 → 11/04/2018

Number of participants: 6

Phd Student:
Zhang, Jin (Intern)

Supervisor:
Voorhees, Peter (Ekstern)

Main Supervisor:
Poulsen, Henning Friis (Intern)
Determination of material parameters by comparison of 3D simulations and 3D experiments
Project: PhD

**Novel Methodologies for Analysis and Interpretation of X-ray Free Electron Lasers Measurements of Structural Dynamics During Chemical Reactions**

Department of Physics  
**Period:** 01/02/2015 → 22/02/2018  
**Number of participants:** 4  
**Phd Student:** Hansen, Frederik Beyer Kjær (Intern)  
**Supervisor:** Haldrup, Kristoffer (Intern)  
**Møller, Klaus Braagaard (Intern)**  
**Main Supervisor:** Nielsen, Martin Meedom (Intern)

**Financing sources**  
**Source:** Internal funding (public)  
**Name of research programme:** Institut stipendie (DTU)  
**Project:** PhD

**Development and characterisation of radiation sensitive polymers for 3D dosimetry of x-rays**

Department of Physics  
**Period:** 01/01/2015 → 16/05/2018  
**Number of participants:** 7  
**Phd Student:** Bernal Zamorano, Maria del Rocio (Intern)  
**Supervisor:** Andersen, Claus E. (Intern)  
**Helt-Hansen, Jakob (Intern)**  
**Main Supervisor:** Lindvold, Lars René (Intern)  
**Examiner:** Jensen, Mikael (Intern)  
**Bäck, Sven (Ekstern)**  
**Sharpe, Peter (Ekstern)**

**Financing sources**  
**Source:** Internal funding (public)  
**Name of research programme:** Institut stipendie (DTU)  
**Project:** PhD

**In vitro dose rate effects of internal and external exposure to ionizing radiation**

Department of Physics  
**Period:** 01/01/2015 → 31/12/2017  
**Number of participants:** 6  
**Phd Student:**
New technology for fast localization and characterization of faults in solar cell systems
The purpose is to develop and demonstrate a new efficient and flexible technology for fault localization/diagnosis in PV systems. The technology is aimed at the growing PV service market. Measurements can be carried out at the string level, and O&M costs are minimized. At the same time performance is optimized and the cost of energy is lowered.

Department of Photonics Engineering
Diode Lasers and LED Systems
Optical Microsensors and Micromaterials
Experimental Surface and Nanomaterials Physics
Department of Micro- and Nanotechnology
Silicon Microtechnology
EmaZys Technologies
Kenergy
Aalborg University
Period: 01/01/2015 → 31/01/2016
Number of participants: 4
Solar Cells, Solar Energy, Characterization
Project participant:
Poulsen, Peter Behrensdorff (Intern)
Thorsteinsson, Sune (Intern)
Schou, Jørgen (Intern)
Hansen, Ole (Intern)

Financing sources
Source: Public research programme (public)
Name of research programme: EUDP
Amount: 8,209,548.00 Danish Kroner
Project:
Hydrodynamics of small Marine Organisms
Department of Physics
Period: 15/12/2014 → 11/04/2018
Number of participants: 7
Phd Student:
Dölger, Julia (Intern)
Supervisor:
Bohr, Tomas (Intern)
Kjærboe, Thomas (Intern)
Main Supervisor:
Andersen, Anders Peter (Intern)
Examiner:
Jensen, Kaare Hartvig (Intern)
Koehl, Mimi A. R. (Ekstern)
Lauga, Eric (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet
Project: PhD

Ice lithography for large-scale sub-10 nm patterning
Department of Physics
Period: 15/12/2014 → 16/05/2018
Number of participants: 6
Phd Student:
Tiddi, William (Intern)
Supervisor:
Han, Anpan (Intern)
Main Supervisor:
Beleggia, Marco (Intern)
Examiner:
Yvind, Kresten (Intern)
Hagen, Cornelis Wouter Kees (Ekstern)
Nouvertné, Frank (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Improved collection efficiency of photons from NV centers for applications in magnetometry
Department of Physics
Period: 15/12/2014 → 15/09/2018
Number of participants: 3
Phd Student:
Ahmadi, Sepehr (Intern)
Supervisor:
Huck, Alexander (Intern)
Main Supervisor:
Andersen, Ulrik Lund (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Magnetic nanoparticle-materials: The structure-propety link of magnetic multi-core particles
Department of Physics
Period: 15/12/2014 → 19/04/2018
Number of participants: 6
Phd Student:
Kure, Mathias (Intern)
Supervisor:
Lefmann, Kim (Intern)
Main Supervisor:
Frandsen, Cathrine (Intern)
Examiner:
Schiøtz, Jakob (Intern)
Folven, Erik (Ekstern)
Nordblad, Per (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

**Analysis of low-energy gamma-ray emitting radionuclides in the environment**
Department of Physics
Period: 01/12/2014 → 17/01/2018
Number of participants: 6
Phd Student:
Markovic, Nikola (Intern)
Supervisor:
Nielsen, Sven Poul (Intern)
Main Supervisor:
Roos, Per (Intern)
Examiner:
Jensen, Mikael (Intern)
Hult, Mikael Bernt Åke (Ekstern)
Murray, Andrew Sean (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

**Development of measurement protocols for quantum magnetometry**
Department of Physics
Period: 01/12/2014 → 09/02/2018
Number of participants: 7
Phd Student:
Stark, Alexander (Intern)
Supervisor:
Huck, Alexander (Intern)
Jelezko, Fedor (Ekstern)
Main Supervisor:
Andersen, Ulrik Lund (Intern)
Examiner:
Wubs, Martijn (Intern)
Balasubramanian, Gopalakrishnan (Ekstern)
Maletinsky, Patrick (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering

**Relations**
Publications:
Development of measurement protocols for quantum magnetometry
Project: PhD

**Frontier Studies of Metal Thin-films: Deposition and Characterization**
Department of Physics
Period: 01/12/2014 → 11/04/2018
Number of participants: 7
Phd Student:
Structure-activity relations in novel catalysts for decentralized methanol synthesis

Department of Physics
Period: 01/12/2014 → 01/06/2018
Number of participants: 3
PhD Student:
Spiga, Cristiano (Intern)
Supervisor:
Chorkendorff, Ib (Intern)
Main Supervisor:
Damsgaard, Christian Danvad (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Is OSL dating using rock clast surfaces more widely applicable and accurate than the classical approach using sand?

Department of Physics
Period: 15/11/2014 → 31/03/2021
Number of participants: 2
PhD Student:
Freiesleben, Trine Holm (Intern)
Main Supervisor:
Thomsen, Kristina Jørkov (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Optical Scanner for read out and visualisation of 3D dose profiles in radiation sensitive polymers

Department of Physics
Period: 15/11/2014 → 16/05/2018
Number of participants: 6
PhD Student:
Sanders, Nicolai Højer (Intern)
Supervisor:
Andersen, Claus E. (Ekstern)
Main Supervisor:
Lindvold, Lars René (Intern)
Examiner:
Lauritzen, Bent (Intern)
Balling, Peter (Ekstern)
Bäck, Sven (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

**Structural dynamics of water solvation, studied with theoretical approaches and ultrafast X-ray methods**

Department of Physics
Period: 15/11/2014 → 11/04/2018
Number of participants: 7
Phd Student:
Vester, Peter (Intern)
Supervisor:
Haldrup, Kristoffer (Intern)
Møller, Klaus Braagaard (Intern)
Main Supervisor:
Nielsen, Martin Meedom (Intern)
Examiner:
Andreasen, Jens Wenzel (Intern)
Abela, Rafael (Ekstern)
Larsen, Sine (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

**Computational screening of new inorganic materials for high-efficiency solar cells**

Department of Physics
Period: 01/11/2014 → 17/01/2018
Number of participants: 6
Phd Student:
Kuhar, Korina (Intern)
Supervisor:
Thygesen, Kristian Sommer (Intern)
Main Supervisor:
Jacobsen, Karsten Wedel (Intern)
Examiner:
Schiøtz, Jakob (Intern)
Hautier, Geoffroy (Ekstern)
Jónsson, Hannes (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)

**Relations**

**Publications:**
Computational screening of new inorganic materials for highly efficient solar energy conversion
Project: PhD

**Electron Microscopy of Catalyst Nanoparticles**

Department of Physics
Period: 01/11/2014 → 17/01/2018
Number of participants: 7
Phd Student:
Liu, Pei (Intern)
Supervisor:
Schiøtz, Jakob (Intern)
Wagner, Jakob Birkedal (Intern)
Main Supervisor:
Hansen, Thomas Willum (Intern)
Examiner:
Kadkhodazadeh, Shima (Intern)
Pérez Omil, Jose Antonio (Ekstern)
Walmsley, John Charles (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering

Relations
Activities:
16th International Congress on Catalysis
Publications:
Environment-Dependent Surface Dynamics of Supported Gold Nanoparticles Studied by High-Resolution Transmission Electron Microscopy
Project: PhD

X-ray Tracking of Electronic and Structural Dynamics During Chemical Reactions Using Free Electron Lasers

Department of Physics
Period: 01/11/2014 → 12/04/2018
Number of participants: 7
Phd Student:
Laursen, Mads (Intern)
Supervisor:
Haldrup, Kristoffer (Intern)
Møller, Klaus Braagaard (Intern)
Main Supervisor:
Nielsen, Martin Meedom (Intern)
Examiner:
Poulsen, Henning Friis (Intern)
Feidenhans'l, Robert Krarup (Intern)
Milne, Christopher J. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Coarsening of polycrystalline structures

Department of Physics
Period: 01/10/2014 → 13/06/2018
Number of participants: 5
Phd Student:
Ahl, Sonja Rosenlund (Intern)
Main Supervisor:
Poulsen, Henning Friis (Intern)
Examiner:
Haldrup, Kristoffer (Intern)
Bernier, Joel Vincent (Ekstern)
Ill, Carl E Krill (Ekstern)

Financing sources
Quantum spin glasses
Department of Physics
Period: 15/09/2014 → 16/11/2018
Number of participants: 3
Phd Student:
Fogh, Ellen (Intern)
Supervisor:
Toft-Petersen, Rasmus (Intern)
Main Supervisor:
Christensen, Niels Bech (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

The influence of neutral particles on blob filaments in magnetically confined plasma
Department of Physics
Period: 15/09/2014 → 23/04/2018
Number of participants: 7
Phd Student:
Thrysøe, Alexander Simon (Intern)
Supervisor:
Madsen, Jens (Intern)
Rasmussen, Jens Juul (Intern)
Main Supervisor:
Naulin, Volker (Intern)
Examiner:
Salewski, Mirko (Intern)
Ciraolo, Guido (Ekstern)
Tala, Tuomas (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet
Project: PhD

Advanced methods for total energy calculations of complex materials
Department of Physics
Period: 01/09/2014 → 15/11/2017
Number of participants: 5
Phd Student:
Schmidt, Per Simmendefeldt (Intern)
Main Supervisor:
Thygesen, Kristian Sommer (Intern)
Examiner:
Schietz, Jakob (Intern)
Grüneis, Andreas (Ekstern)
Rohlfing, Michael (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Relations
Publications:
Development and application of advanced methods for electronic structure calculations
Project: PhD

Characterization of Nanomaterials with Experimental Measurements and Atomistic Simulations
Department of Physics
Period: 01/09/2014 → 15/11/2017
Number of participants: 6
Phd Student:
Larsen, Peter Mahler (Intern)
Supervisor:
Schmidt, Søren (Intern)
Main Supervisor:
Schiøtz, Jakob (Intern)
Examiner:
Thygesen, Kristian Sommer (Intern)
Ferrando, Riccardo (Ekstern)
Goedecker, Stefan (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)

Relations
Publications:
Structural Analysis Algorithms for Nanomaterials
Project: PhD

Modelling the environmental dependent structure of catalyst nanoparticles
Department of Physics
Period: 01/09/2014 → 09/02/2018
Number of participants: 6
Phd Student:
Madsen, Jacob (Intern)
Supervisor:
Hansen, Thomas Willum (Intern)
Main Supervisor:
Schiøtz, Jakob (Intern)
Examiner:
Jacobsen, Karsten Wedel (Intern)
Nellist, Peter (Ekstern)
Peterson, Andrew (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering

Relations
Publications:
Quantitative Image Simulation and Analysis of Nanoparticles
Project: PhD

Particle-particle Interactions in Microfluidics
Department of Physics
Period: 15/08/2014 → 15/11/2017
Number of participants: 5
Phd Student:
Theory of nonlinear acoustic forces acting on fluids and particles in microsystems

Department of Physics
Period: 15/08/2014 → 11/04/2018
Number of participants: 5
Phd Student:
Karlsen, Jonas Tobias (Intern)
Main Supervisor:
Bruus, Henrik (Intern)
Examiner:
Thomsen, Erik Vilain (Intern)
Drinkwater, Bruce W. (Ekstern)
Thomas, Jean-Louis (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)

Relations
Publications:
Theory of nonlinear acoustic forces acting on fluids and particles in microsystems
Project: PhD

Kemien, der kan alt – interaktivt læringsspil

Department of Physics
Period: 02/06/2014 → 03/07/2017
Number of participants: 4
Project participant:
Lanng, Maria (Intern)
Søgaard, Søren Schultz (Ekstern)
Project Manager, organisational:
Toldbod, Ida (Ekstern)
Project Manager, academic:
Zwisler, Laila (Intern)

Development of Novel Catalysts for HT-PEM Fuel Cells

Department of Physics
Period: 01/05/2014 → 16/08/2017
Number of participants: 7
Phd Student:
Jensen, Kim Degn (Intern)
Supervisor:
Escribano, Maria Escudero (Intern)
Stephens, Ifan (Intern)
Main Supervisor:
Chorkendorff, Ib (Intern)
Examiner:
Chakraborty, Debasish (Intern)
Arenz, Matthias (Ekstern)
Hoster, Harry Ernst (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering

Relations
Publications:
Electrochemical Insights into Platinum Catalysts for Fuel Cells
Project: PhD

Characterisation and modelling of crystallographic orientation changes at the grain scale during plastic deformation
Department of Mechanical Engineering
Materials and Surface Engineering
Department of Physics
Neutrons and X-rays for Materials Physics
Period: 01/04/2014 → 31/03/2017
Number of participants: 3
Project participant:
Juul, Nicolai Ytterdal (Intern)
Winther, Grethe (Intern)
Oddershede, Jette (Intern)

Relations
Parent project:
Multi-scale material models for smart metal forming
Related projects:
Mechanical and microstructural transients after strain path changes in metal forming
Project

Novel catalysts based on bimetallic deposited clusters tested in gas-flow microreactors (ESR4), CATSENSE
Department of Physics
Period: 01/04/2014 → 16/08/2017
Number of participants: 5
Phd Student:
Sebök, Béla (Intern)
Main Supervisor:
Chorkendorff, Ib (Intern)
Examiner:
Horch, Sebastian (Intern)
Lievens, Peter (Ekstern)
Yin, Jinlong (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Marie Curie (EU-stipendium)

Relations
Productions of biologically relevant radionuclides to be used as diagnostics and therapeutics

Department of Physics
Period: 01/03/2014 → 25/09/2017
Number of participants: 6
Phd Student:
Fonslet, Jesper (Intern)
Supervisor:
Severin, Gregory (Intern)
Main Supervisor:
Jensen, Mikael (Intern)
Examiner:
Lindvold, Lars René (Intern)
Engle, Jonathan Ward (Ekstern)
Hemmingsen, Lars Bo Stegeager (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Anden EU-finansiering

Relations
Publications:
Production and utilization of unconventional radiometals for advanced diagnostics and therapy

Heterojunction Silicon Solar Cells
One of the most severe challenges man is facing today is to fulfill the need for energy without harmful environmental consequences. This complicated, grand challenge must be met by a wide range of solutions; among these are more efficient use of resources and replacement of fossil fuels by renewable energy sources. Any sustainable, renewable energy system must directly or indirectly rely on solar energy. Photovoltaic or solar cells are already efficient and reliable sources of electricity from solar light, but even though the cost has decreased significantly in recent years, solar cells are still far too costly for a competitive production of bulk grid power. The challenge within the solar cell field is thus to reduce the costs involved in solar cell production without sacrificing efficiency and reliability; actually, the efficiency should better improve towards 25% or more, since the cell efficiency strongly affects the overall economy of a solar cell power plant.

Currently, most of the solar cell market is based on 180-300 micrometer thick crystalline silicon wafers, and approximately 50% of the cost is due to the cost of the material. To reduce material costs thin film cells are promising alternatives, but a limitation in thin film solar cell technologies is that the absorbance of light is quite weak in particular for indirect band gap materials like silicon. This limitation may be lifted by application of photon trapping strategies that can increase the absorptivity of thin photo-absorbers by orders of magnitude at longer wavelengths. Another proved approach in solar cell optimization is carrier selective contacts, such as conventional amorphous silicon, or wide bandgap metal oxide semiconductor.

In this project, we will explore several new ideas for novel silicon-based solar cells to develop efficient solar cells that can be fabricated in a low thermal budget, low-cost fabrication procedure using only abundant elements. The main photo-absorber will be lightly doped p-type silicon (1.12 eV band gap) with a thin n-type TiO₂ (3.2 eV band gap) film on top. This structure forms a p-n heterojunction that effectively separates the photo-generated electron hole-pairs, since the titania and silicon conduction bands are aligned facilitating electron transport, while a ~2 eV energy barrier will prevent hole transport. The electrons transported through the titania to the surface will be conducted laterally by a metal grid or continuous transparent conductive oxides such as Aluminum Zinc Oxide (AZO) with high conductivity, highly transparent (loss 10 %) electrode layer. On the backside, silicon will be coated with complementary to TiO₂ thin film of NiO. NiO is p-type wide bandgap (3.6 eV) semiconductor. In connection to Si it will form p-p isotype hetrojunction with excellent valence band matching, and creating hole conducting and electron blocking layer. A back contact will be formed using a high work-function metal to form additional a potential barrier against electron transport, while the holes are easily conducted to the metal. This basic structure will be combined with micro and nanostructuring of the silicon surface prior to fabrication to form a light trapping structure. All fabrication procedures may be done at temperatures close to room temperature with a maximum of ~200°C necessary in a single step, and thus the thermal budget becomes unusually low. At the same time, a high open circuit voltage for the structure is expected due to the efficient carrier separation in the structure.

The overall project will have four main research phases. In the first phase of the project, the basic TiO₂-Si heterostructure will be optimized on planar silicon wafers. Here the focus will be on the development of optimized fabrication procedures that results in high-performance junctions and efficient lateral transport. In this phase of the project, we also want to
fabricate silicon alumina-titania heterostructures. Alumina has properties similar to titania: a wide bandgap and transparency to visible wavelengths, hole transport blocking and passivation of a silicon surface. In the process, alumina will be deposited on top of silicon and then the lithographic windows will be opened for titania deposition and formation of localized titania-silicon heterojunctions. On top of titania areas aluminum contacts will be introduced. It is planned to fabricate and test such structures since they have a potential to show both high open circuit voltage and short circuit current. Other metal with close by work function will be tested to minimize current blocking effects in diode structure. In the second stage, NiO-Si isotype heterostructure will be tested and optimized to meet the best ohmic (hole conductive) properties. We will fabricate and characterize NiO-Si structure similar to TiO$_2$-Si structure. Next micro- and nanostructured silicon surfaces, including "Black silicon", for light trapping will be developed and characterized. In this stage, nanostructured surfaces should be optimized to obtain the lowest surface recombination velocity in comparison to plain silicon. Then the optimized heterostructure cell fabrication procedure will be ported to these structures. Finally, after the previous three stages will be developed, different solar cell architectures will be tested for solar cell fabrication and characterization. We consider Pasha, HIT and IBC architecture as the most promising for solar cell test since they showed the world records of efficiencies for conventional silicon solar cells.

Department of Micro- and Nanotechnology
Silicon Microtechnology
Department of Physics
Experimental Surface and Nanomaterials Physics
Nanoprobes
Nanointegration
Project ID: 3315
Project participant:
Plakhotnyuk, Maksym (Intern)
Supervisor:
Schmidt, Michael Stenbæk (Intern)
Booth, Tim (Intern)
Main Supervisor:
Hansen, Ole (Intern)

Relations
Activities:
6th Symposium on Carbon and Related Nanomaterials
Fraunhofer Center for Silicon Photovoltaics (CSP)
Discovering Challenges in Fabrication of Nanostructured c-Si Solar Cells with Metal Oxides Carrier Selective Contacts
European Advanced Material Congress
26th International Photovoltaic Science and Engineering Conference

Publications:
Phosphorous Doping of Nanostructured Crystalline Silicon
Low surface damage dry etched black silicon
Lifetime of Nano-Structured Black Silicon for Photovoltaic Applications
Graphene transfer on highly corrugated black silicon surface
TiO$_2$-Si solar cells with carrier selective contacts and low temperature processing
Behind the Nature of Titanium Oxide Excellent Surface Passivation and Carrier Selectivity of c-Si
Phosphorous Doping of Nanostructured Crystalline Silicon
Hole Selective NiO Contact for Silicon Solar Cells
Enhanced Passivation And Characterization Of Titania Silicon Heterojunction With Tunneling Oxide Interlayers

Discovering Challenges in Fabrication of Nanostructured c-Si Solar Cells with Metal Oxides Carrier Selective Contacts

\textbf{Investigations of Nanoparticles for Sustainable Catalysis}
Department of Physics
Period: 15/02/2014 → 25/09/2017
Number of participants: 5
Phd Student:
Bodin, Anders (Intern)
Main Supervisor:
Chorkendorff, Ib (Intern)
Examiner:
Chakraborty, Debasish (Intern)
Jaramillo, Thomas Francisco (Ekstern)
Vajda, Stefan (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)

Relations
Publications:
Synthesis of Nanoparticle Model Systems for Sustainable Catalysis by Gas Aggregation
Project: PhD

Multi-scale material models for smart metal forming
Analysis of deformation-induced intragranular orientation spread in IF-steel by a combination of 3DXRD and crystal plasticity

Department of Mechanical Engineering
Materials and Surface Engineering
Department of Physics
Neutrons and X-rays for Materials Physics
Manufacturing Engineering
DTU Admission Course
University of Illinois
Period: 01/02/2014 → 31/07/2017
Number of participants: 5
Acronym: MulMatMod
Number of related Ph.D. students: 2
Project participant:
Winther, Grethe (Intern)
Oddershede, Jette (Intern)
Bay, Niels Oluf (Intern)
Juul, Nicolai Ytterdal (Intern)
Jensen, Mikkel Ravn Boye (Intern)

Relations
Related projects:
Characterisation and modelling of crystallographic orientation changes at the grain scale during plastic deformation
Mechanical and microstructural transients after strain path changes in metal forming
Activities:
Hierarchical microstructures in metals due to dislocation-mediated plasticity
Grain-scale investigations of deformation and surface treatment of stainless steel
Intragranular orientation spread induced by grain interaction
Parallel evolution of deformation textures and dislocation boundaries
Combining crystal plasticity and dislocation theory to model dislocation boundary characteristics
Intragranular orientation spread induced by grain interaction
Deformation-induced intragranular orientation spread in ferrite investigated by 3DXRD and forward modeling
Measured Resolved Shear Stresses on Slip Systems in Austenitic Steel Grains
Analysis of grain-scale experimental data in a crystal plasticity framework
Analysis of deformation-induced intragranular orientation spread in IF-steel by a combination of 3DXRD and crystal plasticity

Publications:
Deformation-induced orientation spread in individual bulk grains of an interstitial-free steel
Analysis of deformation-induced intragranular orientation spread in IF-steel by a combination of 3DXRD and crystal plasticity

Project

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 Bjørholm (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

Density functional theory studies of hydodesulfurization

Department of Physics
Period: 01/01/2014 → 22/02/2017
Number of participants: 7
Phd Student:
Šaric, Manuel (Intern)
Supervisor:
Moses, Poul Georg (Intern)
Rossmeisl, Jan (Intern)
Main Supervisor:
Jacobsen, Karsten Wedel (Intern)
Examiner:
Stephens, Ifan (Intern)
Lopez, Nuria (Intern)
Behrens, Malte (Ekstern)

Financing sources
Relations
Publications:
Catalyst design for clean and efficient fuels
Project: PhD

Enabling Ultra Deep Hydrodesulfurization by Nanoscale Engineering of New Catalysts

Department of Physics
Period: 15/12/2013 → 15/11/2017
Number of participants: 5
Phd Student:
Christoffersen, Ann-Louise Nygård (Intern)
Main Supervisor:
Chorkendorff, Ib (Intern)
Examiner:
Vesborg, Peter Christian Kjærgaard (Intern)
Lauritsen, Jeppe Vang (Ekstern)
Skoglundh, Bo Magnus (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering

Relations
Publications:
Enabling Ultra Deep Hydrodesulfurization by Nanoscale Engineering of New Catalysts

Controlling Functionality in Biological and Biologically-Inspired Materials

Department of Physics
Period: 01/12/2013 → 21/05/2015
Number of participants: 2
Phd Student:
Wood, Elizabeth Baker (Intern)
Main Supervisor:
Hélix-Nielsen, Claus (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Offentlig finansiering

Understanding defect related luminescence processes in wide bandgap materials using low temperature multi-spectroscopic techniques.

Department of Physics
Period: 01/11/2013 → 14/06/2017
Number of participants: 6
Phd Student:
Prasad, Amit Kumar (Intern)
Supervisor:
Lapp, Torben (Intern)
Main Supervisor:
Jain, Mayank (Intern)
Examiner:
Buylaert, Jan-Pieter (Intern)
Tsukamoto, Sumiko (Ekstern)
Lichtenberg, Jakob (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)

**Relations**
Publications:
Understanding defect related luminescence processes in wide bandgap materials using low temperature multi-spectroscopic techniques
Project: PhD

**Sizing of Microparticles from Angular Scattering Ratio**
This was the pilot project for DTU Compute's 'Number Cruncher Bootcamps' initiative. The results were presented at DTU's first Foodtech Bazaar, held in Roskilde on October 30 2013.

Department of Applied Mathematics and Computer Science
Scientific Computing

Department of Physics
Dynamical Systems
Period: 22/10/2013 → 23/10/2013
Number of participants: 2
Project participant:
Karamehmedovic, Mirza (Intern)
Project Manager, academic:
Hjorth, Poul G. (Intern)

**Relations**
Publications:
Sizing of Microparticles from Angular Scattering Ratio
Documents:
ratio_4-2
Project

**Environment dependent structure of catalyst nanoparticles**
DFF-FTP Sapere Aude projekt.
Center for Electron Nanoscopy

DTU Danchip
Department of Physics
Period: 01/10/2013 → 31/12/2017
Number of participants: 4
Acronym: DynCat
Project ID: 87039
Project participant:
Hansen, Thomas Willum (Intern)
Schiøtz, Jakob (Intern)
Madsen, Jacob (Intern)
Liu, Pei (Intern)
Project

**Carbon inhibition of the Methanation Reaction on Ni-based Model Catalysts**
Department of Physics
Period: 01/10/2013 → 15/11/2017
Number of participants: 6
Phd Student:
Olesen, Sine Ellemann (Intern)
Electronic Properties of Transition Metal Dichalcogenide Heterostructures

Department of Physics
Period: 15/09/2013 → 12/12/2016
Number of participants: 5
Phd Student:
Latini, Simone (Intern)
Main Supervisor:
Thygesen, Kristian Sommer (Intern)
Examiner:
Jacobsen, Karsten Wedel (Intern)
Gatti, Matteo (Ekstern)
Wehling, Tim Oliver (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Grundforskningsfonden

Relations
Publications:
Excitons in van der Waals Heterostructures: A theoretical study
Project: PhD

Microfluidics of Sugar Transport in Trees and in Biomimetic Devices

Department of Physics
Period: 15/09/2013 → 26/10/2016
Number of participants: 6
Phd Student:
Rademaker, Hanna (Intern)
Supervisor:
Jensen, Kaare Hartvig (Intern)
Main Supervisor:
Bohr, Tomas (Intern)
Examiner:
Jacobsen, Karsten Wedel (Intern)
Clanet, Christophe (Ekstern)
Holbrook, Noel Michele (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet
Relations
Publications:
Microfluidics of sugar transport in plant leaves and in biomimetic devices
Project: PhD

Entanglement Enhanced Quantum Communication and Bio-sensing
Department of Physics
Number of participants: 6
Phd Student:
Jacobsen, Christian Scheffmann (Intern)
Supervisor:
Berg-Sørensen, Kirstine (Intern)
Main Supervisor:
Andersen, Ulrik Lund (Intern)
Examiner:
Huck, Alexander (Intern)
Alléaume, Romain (Ekstern)
Villoresi, Paolo (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.

Relations
Publications:
Quantum Information Protocols with Gaussian States of Light
Project: PhD

First-principles theory of Light-matter interaction in Low-dimensional Materials
Department of Physics
Period: 01/09/2013 → 15/03/2017
Number of participants: 5
Phd Student:
Gjerding, Morten Niklas (Intern)
Main Supervisor:
Thygesen, Kristian Sommer (Intern)
Examiner:
Andersen, Ulrik Lund (Intern)
Peres, Nuno M. R. (Ekstern)
Wirtz, Ludger (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)

Relations
Publications:
Light-matter interaction in low-dimensional materials. A theoretical study
Project: PhD

Further developing the Micro-reactor platform with the aim of developing new catalyst for electrochemical CO2 hydrogenation and synthesizing H2O2 by photo-catalysis.

Department of Physics
Period: 01/09/2013 → 15/11/2017
Number of participants: 6
Phd Student:
Trimarco, Daniel Bøndergaard (Intern)
Global Modelling of Turbulence and Transport in Magnetically Confined Plasma

Department of Physics
Period: 01/09/2013 → 14/06/2017
Number of participants: 7
Phd Student:
Magnussen, Michael Løiten (Intern)
Supervisor:
Madsen, Jens (Intern)
Naulin, Volker (Intern)
Main Supervisor:
Rasmussen, Jens Juul (Intern)
Examiner:
Andersen, Anders Peter (Intern)
Hnat, Bogdan (Ekstern)
Kendl, Alexander (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.

Relations
Publications:
Global numerical modeling of magnetized plasma in a linear device
Project: PhD

Identifying the formation and Optimizing the Active Sites of Pt.M Alloys for the ORR Using Synchrotron Light Facilities

Department of Physics
Period: 01/09/2013 → 12/12/2016
Number of participants: 7
Phd Student:
Pedersen, Anders Filsøe (Intern)
Supervisor:
Nilsson, Anders (Ekstern)
Stephens, Ifan (Intern)
Main Supervisor:
Chorkendorff, Ib (Intern)
Examiner:
Horch, Sebastian (Intern)
Magnussen, Olaf (Ekstern)
Salmeron, Miquel B. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)

Relations
Publications:
Elucidating oxygen electrocatalysis with synchrotron X-rays: PEM fuel cells and electrolyzers
Project: PhD

Quantum Protocols with a Colour Centre in a Microcavity
Department of Physics
Number of participants: 6
Phd Student:
Schäfermeier, Clemens (Intern)
Supervisor:
Huck, Alexander (Intern)
Main Supervisor:
Andersen, Ulrik Lund (Intern)
Examiner:
Berg-Sørensen, Kirstine (Intern)
Treps, Nicolas (Ekstern)
Vitali, David (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.

Relations
Publications:
Quantum enhanced optical sensing
Project: PhD

Synthesis and Testing of new Platinum Based Alloy Catalysts for the Oxygen Reduction Reaction
Department of Physics
Number of participants: 7
Phd Student:
Zamburlini, Eleonora (Intern)
Supervisor:
Escribano, Maria Escudero (Intern)
Stephens, Ifan (Intern)
Main Supervisor:
Chorkendorff, Ib (Intern)
Examiner:
Chakraborty, Debashish (Intern)
Granozzi, Gaetano (Ekstern)
Hjuler, Hans Aage (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering

Relations
Publications:
Pt-based Thin Films as Efficient and Stable Catalysts for Oxygen Electroreduction
Project: PhD
X-ray Tracking of Atomic Motion During Chemical Reactions Using Free Electron Lasers

Department of Physics
Period: 01/09/2013 → 12/12/2016
Number of participants: 7
Phd Student:
Biasin, Elisa (Intern)
Supervisor:
Christensen, Morten (Intern)
Haldrup, Kristoffer (Intern)
Main Supervisor:
Nielsen, Martin Meedom (Intern)
Examiner:
Thygesen, Kristian Sommer (Intern)
Nilsson, Anders (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut, samfinansiering

Relations
Publications:
Structural dynamics of solvated metal complexes with anisotropy-enhanced X-ray scattering
Project: PhD

Plasmon supported optical nanosensors and their application for probing artificial and biological micro- and nanochannels

Department of Physics
Period: 01/08/2013 → 26/10/2016
Number of participants: 6
Phd Student:
Palanco, Marta Espina (Intern)
Supervisor:
Hélix-Nielsen, Claus (Intern)
Main Supervisor:
Berg-Sørensen, Kirstine (Intern)
Examiner:
Andersen, Ulrik Lund (Intern)
Dholakia, Kishan (Ekstern)
Kleinschmidt, Jörg Helmut (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.

Relations
Publications:
Optical sensors and their applications for probing biological systems
Project: PhD

Quantification of radiation induced DNA damage following intracellular Auger cascade

Department of Physics
Period: 01/08/2013 → 25/09/2017
Number of participants: 5
Phd Student:
Fredericia, Nina Pil Mentegaard (Intern)
Main Supervisor:
Jensen, Mikael (Intern)
Examiner:
Andersen, Claus E. (Intern)
Hansen, Steen Laugesen (Ekstern)
Kriehuber, Ralf (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Offentlig finansiering

Relations
Publications:
Quantification of Radiation-induced DNA Damage following intracellular Auger-Cascades
Project: PhD

DFT-Simulations of low temperature fuel cells catalysis
Department of Physics
Period: 15/05/2013 → 25/08/2016
Number of participants: 6
Phd Student:
Hansen, Martin Hangaard (Intern)
Supervisor:
Rossmeisl, Jan (Intern)
Main Supervisor:
Thygesen, Kristian Sommer (Intern)
Examiner:
Jacobsen, Karsten Wedel (Intern)
Groß, Axel (Ekstern)
Koper, Marcus Theodorus Maria (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering

Relations
Publications:
Atomic-scale Modelling of Electro-catalytic Surfaces and Dynamic Electrochemical Interfaces
Project: PhD

Evaluation of optical surface scanning of mammary cancer patients for improved radiotherapy
Department of Physics
Period: 01/04/2013 → 13/06/2018
Number of participants: 7
Phd Student:
Bekke, Susanne Nørring (Intern)
Supervisor:
Behrens, Claus F. (Ekstern)
Mahmood, Faisal (Ekstern)
Main Supervisor:
Andersen, Claus E. (Intern)
Examiner:
Lindvold, Lars René (Intern)
Eilstrem, Ulrik Vindelev (Ekstern)
McNair, Helen Anne (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 FUU, 1/3 inst 1/3 Andet
Project: PhD
Multi-scale mapping of strain mechanisms in lead-free piezoceramics

Department of Physics
Period: 15/03/2013 → 22/06/2016
Number of participants: 6
Phd Student:
Majkut, Marta (Intern)
Supervisor:
Oddershede, Jette (Intern)
Main Supervisor:
Schmidt, Søren (Intern)
Examiner:
Poulsen, Henning Friis (Intern)
Clausen, Bjørn (Intern)
Grant Webber, Kyle (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Microreactor measurement of catalytic activity of mass selected nanoparticles

Department of Physics
Period: 01/03/2013 → 25/08/2016
Number of participants: 6
Phd Student:
Riedel, Jakob Nordheim (Intern)
Main Supervisor:
Chorkendorff, Ib (Intern)
Examiner:
Stephens, Ifan (Intern)
Stephens, Ifan (Intern)
Quaade, Ulrich (Intern)
Quaade, Ulrich (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Grundforskningsfonden

Relations
Publications:
μ-reactor measurements of catalytic activity of mass selected nano-particles
Project: PhD

3D Neutron Diffraction (3DND) methodology

Department of Physics
Period: 15/02/2013 → 23/09/2016
Number of participants: 8
Phd Student:
Cereser, Alberto (Intern)
Supervisor:
Hall, Stephen A. (Ekstern)
Steuwer, Axel (Ekstern)
Strobl, Markus (Ekstern)
Main Supervisor:
Schmidt, Søren (Intern)
Examiner:
Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 FUU, 1/3 inst 1/3 Andet

Relations
Publications:
Time-of-flight 3D Neutron Diffraction for Multigrain Crystallography
Project: PhD

FTP-PIEZO Multi-scale mapping of strain mechanisms in lead-free piezoceramics
Department of Physics
Neutrons and X-rays for Materials Physics
University of New South Wales
Period: 01/01/2013 → 14/03/2016
Number of participants: 3
Project participant:
Oddershede, Jette (Intern)
Schmidt, Søren (Intern)
Phd Student:
Majkut, Marta (Intern)

Relations
Related projects:
Multi-scale mapping of strain mechanisms in lead-free piezoceramics
Activities:
Materials characterisation tools towards lead-free piezoceramics
Strain Mechanisms in Polycrystalline BaTiO3 Measured at the Single Grain Level during In-Situ Electrical Poling
Three-Dimensional X-ray Diffraction (3DXRD) microscopy for studying strain evolution in piezoelectric domain structures and deformation induced twinning
Three-Dimensional X-ray Diffraction (3DXRD) microscopy for studying dynamics in polycrystalline materials
Quantitative grain-scale ferroelectric domain volume fractions and domain switching strains measured by 3DXRD during in situ electrical poling
Strain Mechanisms in Polycrystalline BaTiO3 Measured at the Single Grain Level during In-Situ Electrical Poling
Three-Dimensional X-ray Diffraction (3DXRD) microscopy for studying dynamics in polycrystalline materials
Three-Dimensional X-ray Diffraction (3DXRD) microscopy for in situ studies of polycrystalline materials
Publications:
Maximising electro-mechanical response by minimising grain-scale strain heterogeneity in phase-change actuator ceramics
The effect of inter-granular constraints on the response of polycrystalline piezoelectric ceramics at the surface and in the bulk
Mapping of strain mechanisms in barium titanate by three-dimensional X-ray diffraction
Heterogeneous grain-scale response in ferroic polycrystals under electric field
Quantitative grain-scale ferroic domain volume fractions and domain switching strains from three-dimensional X-ray diffraction data
Project

Ny familie af katalysatorer til miniaturiserede metanol brændselsceller
Department of Physics
Period: 01/01/2013 → 25/05/2016
Number of participants: 7
Phd Student:
Nanofabrication of Next-Generation X-Ray Optical Components

Department of Physics
Period: 15/12/2012 → 28/04/2016
Number of participants: 7
Phd Student:
Stöhr, Frederik (Intern)
Supervisor:
Hansen, Ole (Intern)
Jensen, Flemming (Intern)
Main Supervisor:
Poulsen, Henning Friis (Intern)
Examiner:
Thomsen, Erik Vilain (Intern)
Franssila, Sami (Ekstern)
Schroer, Christian Gustav (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Synthesis and Investigation of Platinum Based Electrocatalysts

Department of Physics
Period: 15/12/2012 → 25/08/2016
Number of participants: 6
Phd Student:
Knudsen, Brian Peter (Intern)
Supervisor:
Stephens, Ifan (Intern)
Main Supervisor:
Chorkendorff, Ib (Intern)
Examiner:
Chakraborty, Debasish (Intern)
Arenz, Matthias (Ekstern)
Schmidt, Thomas Justus (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)

Relations
Publications:
Synthesis of Platinum Rare Earth Alloy Catalysts for Fuel Cells
Project: PhD

Ab-initio modelling of electronic excitations in nano-structured graphene
Department of Physics
Period: 15/10/2012 → 31/03/2016
Number of participants: 5
Phd Student:
Rasmussen, Filip Anselm (Intern)
Main Supervisor:
Thygesen, Kristian Sommer (Intern)
Examiner:
Brandbyge, Mads (Intern)
Draxl, Claudia (Ekstern)
Hofmann, Philip (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Grundforskningsfonden

Relations
Publications:
First Principles Calculations of Electronic Excitations in 2D Materials
Project: PhD

Electron Micoscopy of Catalyst Nanostructures
Department of Physics
Period: 15/09/2012 → 09/12/2015
Number of participants: 6
Phd Student:
Gardini, Diego (Intern)
Supervisor:
Damsgaard, Christian Danvad (Intern)
Main Supervisor:
Wagner, Jakob Birkedal (Intern)
Examiner:
Kegnæs, Søren (Intern)
Su, Dang Sheng (Ekstern)
Walmsley, John Charles (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Development of monolithic tandem photocatalytic water splitting cell
Department of Physics
Period: 01/09/2012 → 09/12/2015
Number of participants: 7
Phd Student:
Bae, Dowon (Intern)
Supervisor:
Hansen, Ole (Intern)
Vesborg, Peter Christian Kjærgaard (Intern)
Main Supervisor: Chorkendorff, Ib (Intern)
Examiner: Horch, Sebastian (Intern)
Deutsch, Todd G. (Ekstern)
Sivula, Kevin (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Grundforskningsfonden
Project: PhD

Experimental and computational study of advanced moderators for ESS
Department of Physics
Period: 01/09/2012 → 22/02/2017
Number of participants: 7
Phd Student: Schönfeldt, Troels (Intern)
Supervisor: Willendrup, Peter Kjær (Intern)
Zanini, Luca (Ekstern)
Main Supervisor: Lauritzen, Bent (Intern)
Examiner: Jain, Mayank (Intern)
Farhi, Emmanuel (Ekstern)
Filges, Uwe (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 FUU, 1/3 inst 1/3 Andet

Relations
Publications:
Advanced Neutron Moderators for the ESS
Project: PhD

Improved radiotherapy utilizing 3D and 4D ultrasound imaging techniques
Department of Physics
Period: 01/09/2012 → 24/02/2016
Number of participants: 7
Phd Student: Baker, Mariwan (Intern)
Supervisor: Behrens, Claus F. (Ekstern)
Jensen, Jørgen Arendt (Intern)
Main Supervisor: Andersen, Claus E. (Intern)
Examiner: Lauritzen, Bent (Intern)
Elstrøm, Ulrik Vindelev (Ekstern)
Harris, Emma Jane (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Ansat eksternt

Relations
Publications:
Utilizing 3-D and 4-D ultrasound systems to improve radiation treatment of cervix and prostate cancer patients.

**Methods to determine fast-ion distribution functions from multidiagnostic measurements**

Department of Physics  
Period: 01/09/2012 → 09/12/2015  
Number of participants: 6  
Phd Student:  
Jacobsen, Asger Schou (Intern)  
Supervisor:  
Salewski, Mirko (Intern)  
Main Supervisor:  
Naulin, Volker (Intern)  
Examiner:  
Poulsen, Henning Friis (Intern)  
Bindslev, Henrik (Intern)  
Sharapov, Sergei (Ekstern)

**Financing sources**
Source: Internal funding (public)  
Name of research programme: Institut stipendie (DTU) Samf.

**Multi-scale modeling of electrokinetic phenomena in microchannels and nanoporous membranes**

Department of Physics  
Period: 01/09/2012 → 19/11/2015  
Number of participants: 5  
Phd Student:  
Nielsen, Christoffer Peder (Intern)  
Main Supervisor:  
Bruus, Henrik (Intern)  
Examiner:  
Mortensen, N. Asger (Intern)  
Biesheuvel, Maarten (Ekstern)  
Yaroshchuk, Andriy (Ekstern)

**Financing sources**
Source: Internal funding (public)  
Name of research programme: Institut stipendie (DTU) Samf.

**Quantum control of a mechanical system**

Department of Physics  
Period: 01/09/2012 → 21/01/2016  
Number of participants: 5  
Phd Student:  
Kerdoncuff, Hugo (Intern)  
Main Supervisor:  
Andersen, Ulrik Lund (Intern)  
Examiner:  
Hansen, Jern Otto Bindslev (Ekstern)  
Filip, Radim (Ekstern)  
Marquardt, Christoph Dirk (Ekstern)

**Financing sources**
Source: Internal funding (public)  
Name of research programme: Eksternt finsieret virksomhed

Project: PhD
Computational Screening of Energy Materials
Department of Physics
Period: 01/08/2012 → 30/09/2015
Number of participants: 6
Phd Student:
Pandey, Mohnish (Intern)
Supervisor:
Thygesen, Kristian Sommer (Intern)
Main Supervisor:
Jacobsen, Karsten Wedel (Intern)
Examiner:
Schiøtz, Jakob (Intern)
Jónsson, Hannes (Ekstern)
Wahnström, Göran (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 FUU, 1/3 inst 1/3 Andet
Project: PhD

Modeling of level alignment and charge separation at donor/acceptor interfaces
Department of Physics
Period: 01/08/2012 → 23/10/2015
Number of participants: 6
Phd Student:
Ørnsø, Kristian Baruël (Intern)
Supervisor:
Jacobsen, Karsten Wedel (Intern)
Main Supervisor:
Thygesen, Kristian Sommer (Intern)
Examiner:
Vegge, Tejs (Intern)
Boschloo, Gerrit Klaas (Ekstern)
Troisi, Alessandro (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

New Electro-catalysts for oxygen evolution and reduction
Department of Physics
Period: 01/08/2012 → 23/10/2015
Number of participants: 6
Phd Student:
Frydendal, Rasmus (Intern)
Supervisor:
Stephens, Ifan (Intern)
Main Supervisor:
Chorkendorff, Ib (Intern)
Examiner:
Chakraborty, Debasis (Intern)
Strasser, Peter (Ekstern)
Suntivich, Jin (Ekstern)

Financing sources
Zooplankton Fluid Dynamics

Department of Physics
Period: 01/08/2012 → 19/11/2015
Number of participants: 7
Phd Student:
Wadhwa, Navish (Intern)
Supervisor:
Bohr, Tomas (Intern)
Kjørboe, Thomas (Intern)
Main Supervisor:
Andersen, Anders Peter (Intern)
Examiner:
Rasmussen, Jens Juul (Intern)
Humphries, Stuart (Ekstern)
Zhang, Jun (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Shape and activity of nanoparticulate alloys, with special focus on platinum alloys for the oxygen reduction reaction

Department of Physics
Period: 15/07/2012 → 24/02/2016
Number of participants: 7
Phd Student:
Vej-Hansen, Ulrik Grønbjerg (Intern)
Supervisor:
Rossmeisl, Jan (Intern)
Stephens, Ifan (Intern)
Main Supervisor:
Schiøtz, Jakob (Intern)
Examiner:
Vegge, Tejs (Intern)
Curtin, William A. (Ekstern)
Reuter, Karsten (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.
Project: PhD

Theory and design of microsystems for clinical acousto-activated cell sorting

Department of Physics
Period: 15/04/2012 → 19/11/2015
Number of participants: 5
Phd Student:
Tribler, Peter Muller (Intern)
Main Supervisor:
Bruus, Henrik (Intern)
Examiner:
Sørensen, Jens Nørkær (Intern)
Dual, Jürg (Ekstern)
Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Coherent Coupling of a Nitrogen-Vacancy Center to Gap Modes in Integrated Structures

Department of Physics
Period: 01/04/2012 → 13/08/2015
Number of participants: 6
PhD Student:
Israelsen, Niels Møller (Intern)
Supervisor:
Huck, Alexander (Intern)
Main Supervisor:
Andersen, Ulrik Lund (Intern)
Examiner:
Wubs, Martijn (Intern)
Bozhevolnyi, Sergey I. (Intern)
Jelezko, Fedor (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut, samfinansiering
Project: PhD

Synthesis and Test of Anodes for Photocatalytic Water Splitting

Department of Physics
Period: 01/03/2012 → 31/10/2013
Number of participants: 4
PhD Student:
Lilliedal, Mathilde Raad (Intern)
Supervisor:
Hansen, Ole (Intern)
Vesborg, Peter Christian Kjærgaard (Intern)
Main Supervisor:
Chorkendorff, Ib (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 FUU, 1/3 inst 1/3 Andet
Project: PhD

Computational modelling of electron transport at metal-organic interfaces

Department of Physics
Period: 15/02/2012 → 21/09/2015
Number of participants: 5
PhD Student:
Jin, Chengjun (Intern)
Main Supervisor:
Thygesen, Kristian Sommer (Intern)
Examiner:
Jacobsen, Karsten Wedel (Intern)
Pauly, Fabian (Ekstern)
Ratner, Mark A. (Ekstern)

Financing sources
Electrochemical reduction of CO2 at low temperature in PEMFC-type electrolysis cells

Department of Physics
Period: 01/02/2012 → 28/04/2015
Number of participants: 6
Phd Student:
Verdaguer Casadevall, Arnau (Intern)
Supervisor:
Stephens, Ifan (Intern)
Main Supervisor:
Chorkendorff, Ib (Intern)
Examiner:
Horch, Sebastian (Intern)
Kucernak, Anthony R. (Ekstern)
Stamenkovic, Vojislav R. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 FUU, 1/3 inst 1/3 Andet
Project: PhD

Improved radiotherapy for locally advanced Non-Small Cell Lung Carcinoma (NSCLC) patients

Department of Physics
Period: 01/02/2012 → 13/08/2015
Number of participants: 6
Phd Student:
Ottosson, Wiviann (Intern)
Supervisor:
Behrens, Claus F. (Ekstern)
Main Supervisor:
Andersen, Claus E. (Intern)
Examiner:
Lauritzen, Bent (Intern)
Korreman, Stine Sofia (Ekstern)
Sarrut, David (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.
Project: PhD

Fosfat-bioscavengers/biosensorer for osmotisk baseret detektion/ressource-genindvinding

Department of Physics
Period: 01/01/2012 → 31/07/2012
Number of participants: 2
Phd Student:
Junker, Märta Caroline (Intern)
Main Supervisor:
Hélix-Nielsen, Claus (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.
Project: PhD
Theoretical design of abundant and stable oxygen evolution reaction catalysts
Department of Physics
Period: 01/01/2012 → 19/03/2015
Number of participants: 5
Phd Student: Halck, Niels Bendtsen (Intern)
Main Supervisor: Rossmeisl, Jan (Intern)
Examiner: Vegge, Tejs (Intern)
Dau, Holger (Ekstern)
Hellman, Anders (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 FUU, 1/3 inst 1/3 Andet
Project: PhD

Continuous variable quantum metrology and information processing
Department of Physics
Period: 15/12/2011 → 04/03/2015
Number of participants: 5
Phd Student: Berni, Adriano (Intern)
Main Supervisor: Andersen, Ulrik Lund (Intern)
Examiner: Hansen, Jørn Otto Bindslev (Ekstern)
Björk, Gunnar (Ekstern)
Pirandola, Stefano (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Plasmonic supported vibrational spectroscopy for probing biologically relevant molecules and processing
Department of Physics
Period: 01/12/2011 → 28/02/2013
Number of participants: 3
Phd Student: Berthelsen, Mai-Britt Lund Degn (Intern)
Supervisor: Bohr, Henrik (Intern)
Main Supervisor: Kneipp, Katrin (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Preparation and test of abundant and stable OER catalysts
Department of Physics
Period: 01/12/2011 → 04/03/2015
Number of participants: 6
PhD Student:
Paoli, Elisa Antares (Intern)
Supervisor:
Dahl, Søren (Intern)
Main Supervisor:
Chorkendorff, Ib (Intern)
Examiner:
Hansen, Ole (Intern)
Grahl-Madsen, Laila (Ekstern)
Russell, Andrea E. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 FUU, 1/3 inst 1/3 Andet
Project: PhD

Benefit-Risk Assessment in Drug Development
Department of Physics
Period: 30/11/2011 → 30/04/2012
Number of participants: 7
PhD Student:
Sarac, Sinan Bardakci (Intern)
Supervisor:
Colding-Jørgensen, Morten (Ekstern)
Thirstrup, Steffen (Ekstern)
Main Supervisor:
Mosekilde, Erik (Intern)
Examiner:
Lund, Ole (Intern)
Helboe, Per (Ekstern)
Walker, Stuart (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: ErhvervsPhD-ordningen VTU
Project: PhD

Reference-class luminescence dosimetry for radiotherapy
Department of Physics
Period: 15/11/2011 → 31/03/2016
Number of participants: 5
PhD Student:
Buranurak, Siritorn (Intern)
Main Supervisor:
Andersen, Claus E. (Intern)
Examiner:
Lauritzen, Bent (Intern)
Ceberg, Crister (Ekstern)
Chakarova, Roumiana (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Stipendie fra udlandet
Project: PhD

Aberration-corrected transmission electron microscopy of nanoparticle catalysts
Department of Physics
Period: 01/11/2011 → 23/01/2015
Number of participants: 6
Phd Student:
Deiana, Davide (Intern)
Supervisor:
Wagner, Jakob Birkedal (Intern)
Main Supervisor:
Hansen, Thomas Willum (Intern)
Examiner:
Schietz, Jakob (Intern)
Gamez, José Juan Calvino (Ekstern)
Willinger, Marc-Georg (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Development of new photo-catalyst for water splitting and Hydrogenation of CO2
Department of Physics
Period: 01/11/2011 → 23/01/2015
Number of participants: 6
Phd Student:
Malizia, Mauro (Intern)
Supervisor:
Dahl, Søren (Intern)
Main Supervisor:
Chorkendorff, Ib (Intern)
Examiner:
Chakraborty, Debasish (Intern)
Smith, Wilson (Ekstern)
Tilley, David (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 FUU, 1/3 inst 1/3 Andet
Project: PhD

Modelling of ions at the electrochemical interface at the atomic level
Department of Physics
Period: 01/10/2011 → 28/04/2015
Number of participants: 5
Phd Student:
Ahmed, Rizwan (Intern)
Main Supervisor:
Rossmeisl, Jan (Intern)
Examiner:
Schietz, Jakob (Intern)
Moses, Poul Georg (Intern)
Skulason, Egill (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.
Project: PhD

Fundamentale studier af katalytiske modelsystemer: Énkrystaller og nanopartikler
Department of Physics
Theoretical Investigation of Plasmonic Materials using Electronic Structure Methods

Department of Physics
Period: 01/09/2011 → 13/08/2015
Number of participants: 6
Phd Student:
Winther, Kirsten Trøstrup (Intern)
Supervisor:
Jacobsen, Karsten Wedel (Intern)
Main Supervisor:
Thygesen, Kristian Sommer (Intern)
Examiner:
Schietz, Jakob (Intern)
García de Abajo, Francisco J. (Ekstern)
Puska, Martti Juhani (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Fundamental investigations of the methanol catalysts: Nanoparticle dynamics and composition

Department of Physics
Period: 01/08/2011 → 25/05/2016
Number of participants: 7
Phd Student:
Elkjær, Christian Fink (Intern)
Supervisor:
Helveg, Stig (Ekstern)
Sehested, Jens (Intern)
Main Supervisor:
Chorkendorff, Ib (Intern)
Examiner:
Vesborg, Peter Christian Kjærgaard (Intern)
Carlsson, Per-Anders (Ekstern)
Jinschek, Joerg R. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.
Publications:
Fundamental investigations of catalyst nanoparticles
Project: PhD

Integrated quantum sensing with squeezed light
Department of Physics
Period: 01/08/2011 → 19/06/2015
Number of participants: 5
Phd Student:
Hoff, Ulrich Busk (Intern)
Main Supervisor:
Andersen, Ulrik Lund (Intern)
Examiner:
Rottwitt, Karsten (Intern)
Dantan, Aurélien (Ekstern)
Fabre, Claude (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering

Relations
Publications:
Integrated Quantum Optics: Experiments towards integrated quantum-light sources and quantum-enhanced sensing
Project: PhD

Surface science investigations of new Ni-Ga alloys for reduction of CO2 to fuels
Department of Physics
Period: 01/06/2011 → 26/01/2015
Number of participants: 6
Phd Student:
Ulrikkeholm, Elisabeth Therese (Intern)
Supervisor:
Dahl, Søren (Intern)
Main Supervisor:
Chorkendorff, Ib (Intern)
Examiner:
Damsgaard, Christian Danvad (Intern)
Schnadt, Joachim (Ekstern)
Tougaard, Sven Mosbæk (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Simulations and measurements of the three dimensional coherent structures in the Scrape Off Layer of fusion machines
Department of Physics
Period: 01/05/2011 → 09/09/2014
Number of participants: 6
Phd Student:
Yan, Ning (Intern)
Supervisor:
Wan, Baonian (Ekstern)
Main Supervisor:
Naulin, Volker (Intern)
Examiner:
Bohr, Tomas (Intern)
Development of Surface Science equipment for Electro-catalysis measurements in relation to Solar Fuel conversion

Department of Physics
Period: 15/04/2011 → 29/08/2014
Number of participants: 6
Phd Student: Malacrida, Paolo (Intern)
Supervisor: Horch, Sebastian (Intern)
Main Supervisor: Chorkendorff, Ib (Intern)
Examiner: Chakraborty, Debasish (Intern)
Arenz, Matthias (Ekstern)
Roldán Cuenya, Beatriz (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.
Project: PhD

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 electrolyser 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
Development and testing of new exchange-correlation functionals

Department of Physics
Period: 01/02/2011 → 20/03/2014
Number of participants: 6
PhD Student:
Lundgård, Keld Troen (Intern)
Supervisor:
Thygesen, Kristian Sommer (Intern)
Main Supervisor:
Jacobsen, Karsten Wedel (Intern)
Examiner:
Schietz, Jakob (Intern)
Moses, Poul Georg (Intern)
Tkatchenko, Alexandre (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

X-ray studies og dynamical effects in liquids and at interfaces

Department of Physics
Period: 01/01/2011 → 26/08/2014
Number of participants: 5
PhD Student:
Brandt van Driel, Tim (Intern)
Main Supervisor:
Nielsen, Martin Meedom (Intern)
Examiner:
Thygesen, Kristian Sommer (Intern)
Anders, Madsen (Ekstern)
Collet, Eric (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Grundforskningsfonden
Project: PhD

Konstruktion af et høj-strøms, høj-udbytte O-18 vand target til produktion af F-18

Department of Physics
Period: 15/12/2010 → 09/12/2014
Number of participants: 2
PhD Student:
Selective Electrochemical Reduction of Hydrogen-peroxide and Oxidation of Water

Department of Physics
Period: 15/11/2010 → 24/01/2014
Number of participants: 5
Phd Student: Karamad, Mohammadreza (Intern)
Main Supervisor: Rossmeisl, Jan (Intern)
Examiner: Schiøtz, Jakob (Intern)
Lopez, Nuria (Intern)
Peterson, Andrew (Intern)

Electronic-structure simulations of photo-absorptin properties in extended systems

Department of Physics
Period: 01/11/2010 → 24/01/2014
Number of participants: 6
Phd Student: Hüser, Falco Jonas (Intern)
Supervisor: Schiøtz, Jakob (Intern)
Main Supervisor: Thygesen, Kristian Sommer (Intern)
Examiner: Rossmeisl, Jan (Intern)
Aryasetiawan, Ferdi (Ekstern)
Rinke, Patrick (Ekstern)

Production of Solar fuels by electrochemical fixation of nitrogen and CO2

Department of Physics
Period: 01/11/2010 → 23/06/2014
Number of participants: 6
Phd Student: Jovanov, Zarko (Intern)
Supervisor: Stephens, Ifan (Intern)
Main Supervisor: Chorkendorff, Ib (Intern)
Examiner:
Chakraborty, Debasish (Intern)
Bandarenka, Aliaksandr (Intern)
Schmidt, Thomas Justus (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 FUU, 1/3 inst 1/3 Andet
Project: PhD

Interfacial Electron Transfer of Large Transition Metal Complexes in Condensed Matter Environments

Department of Physics
Period: 01/10/2010 → 25/04/2014
Number of participants: 7
Phd Student:
Jónsson, Elvar Örn (Intern)
Supervisor: Thygesen, Kristian Sommer (Intern)
Ulstrup, Jens (Intern)
Main Supervisor:
Jacobsen, Karsten Wedel (Intern)
Examiner: Rossmeisl, Jan (Intern)
Jónsson, Hannes (Ekstern)
Sprik, Michiel (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Adaptive Simulations of Nonlinear Structures in Magnetized Plasma

Department of Physics
Period: 15/09/2010 → 24/10/2014
Number of participants: 4
Phd Student:
Treue, Frederik (Intern)
Supervisor: Engsig-Karup, Allan Peter (Intern)
Evgrafov, Anton (Intern)
Main Supervisor:
Naulin, Volker (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.
Project: PhD

Development of new photo catalyst for efficient removal of ethylene

Department of Physics
Number of participants: 6
Phd Student:
Nielsen, Morten Godtfred (Intern)
Supervisor: Dahl, Søren (Intern)
Main Supervisor:
Chorkendorff, Ib (Intern)
Examiner:
Chakraborty, Debasis (Intern)
Christensen, Leif Højslet (Intern)
Muhler, Martin (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 FUU, 1/3 inst 1/3 Andet
Project: PhD

Optimizing nanoparticles for catalytic reactions
Department of Physics
Period: 15/09/2010 → 09/09/2014
Number of participants: 6
Phd Student:
Nierhoff, Anders Ulrik Fregerslev (Intern)
Supervisor:
Nielsen, Jane Hvolbæk (Intern)
Main Supervisor:
Chorkendorff, Ib (Intern)
Examiner:
Horch, Sebastian (Intern)
Hansen, Poul Lenvig (Ekstern)
Heiz, Ulrich (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Grundforskningsfonden
Project: PhD

Correlation of reactivity on well defined single crystals and mass selected nanoparticles
Department of Physics
Period: 01/09/2010 → 20/03/2014
Number of participants: 6
Phd Student:
Conradsen, Christian Nagstrup (Intern)
Supervisor:
Nielsen, Jane Hvolbæk (Intern)
Main Supervisor:
Chorkendorff, Ib (Intern)
Examiner:
Hansen, Ole (Intern)
Abrams, Billie (Intern)
Hinrichsen, Kai-Olaf (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Grundforskningsfonden
Project: PhD

Magnetske egenskaber af selvorganiserde nanopartikelsystemer
Department of Physics
Period: 15/08/2010 → 24/01/2014
Number of participants: 7
Phd Student:
Brok, Erik (Intern)
Supervisor:
Hansen, Thomas Willum (Intern)
Lefmann, Kim (Intern)
Main Supervisor:
Frandsen, Cathrine (Intern)
Examiner:
Hansen, Mikkel Fougt (Intern)
Schweika, Werner (Ekstern)
vander Zaag, Pieter J. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.
Project: PhD

Electronic-structure description of the hydrogen-assisted selective catalytic reduction of NO in lean-burn exhaust gasses by ammonia

Department of Physics
Period: 01/08/2010 → 30/08/2013
Number of participants: 6
Phd Student:
Khan, Tuhin Suvra (Intern)
Supervisor:
Bligaard, Thomas (Intern)
Main Supervisor:
Rossmeisl, Jan (Intern)
Examiner:
Stephens, Ifan (Intern)
Hellman, Anders (Ekstern)
Kitchin, John (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Computational search for new light harvesting materials for solar-to-fuel energy conversion

Department of Physics
Period: 01/06/2010 → 26/09/2013
Number of participants: 6
Phd Student:
Castelli, Ivano Eligio (Intern)
Supervisor:
Thygesen, Kristian Sommer (Intern)
Main Supervisor:
Jacobsen, Karsten Wedel (Intern)
Examiner:
Schiatz, Jakob (Intern)
Marzari, Nicola (Ekstern)
Pedersen, Thomas Garm (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Theoretical description of electrochemical co2 reduction

Department of Physics
A quantitative description of subcutaneous injections: from needle to clinical effect

Department of Physics
Period: 01/05/2010 → 12/12/2013
Number of participants: 8

Phd Student:
Rasmussen, Christian Hove (Intern)

Supervisor:

Colding-Jørgensen, Morten (Ekstern)
Mosekilde, Erik (Intern)
Thirstrup, Steffen (Ekstern)

Main Supervisor:
Knudsen, Carsten (Intern)
Examiner:
Berg-Sørensen, Kirstine (Intern)
Frøkjær, Sven (Ekstern)
Rowland, Malcolm (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: ErhvervsPhD-ordningen VTU
Project: PhD

Shape and reactivity of clusters and nanoparticles

Department of Physics
Period: 01/05/2010 → 24/01/2014
Number of participants: 6

Phd Student:
Brodersen, Simon Hedegaard (Intern)

Supervisor:

Nielsen, Jane Hvolbæk (Intern)

Main Supervisor:
Schiotz, Jakob (Intern)
Examiner:
Vegge, Tejs (Intern)
Fortunelli, Alessandro (Ekstern)
Grabow, Lars (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Electrochemical Fixation of Carbon Dioxide to Fuels

Department of Physics
Period: 01/04/2010 → 26/09/2013
Number of participants: 6
Phd Student:
Varela Gasque, Ana Sofia (Intern)
Supervisor:
Nielsen, Jane Hvolbæk (Intern)
Main Supervisor:
Chorkendorff, Ib (Intern)
Examiner:
Hansen, Ole (Intern)
Cuesta, Angel (Ekstern)
Koper, Marcus Theodorus Maria (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

H2 assisteret lavtemperatur SCR
Department of Physics
Period: 01/04/2010 → 30/08/2013
Number of participants: 5
Phd Student:
Fogel, Sebastian (Intern)
Supervisor:
Gabrielsson, Pär (Ekstern)
Main Supervisor:
Chorkendorff, Ib (Intern)
Examiner:
Chakraborty, Debasish (Intern)
Arve, Kalle Ilmari (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Ansat eksternt
Project: PhD

Interplay of structure, magnetism and functionality in high-temperature superconductors and CoCl salts
Department of Physics
Period: 01/04/2010 → 30/09/2013
Number of participants: 7
Phd Student:
Larsen, Jacob (Intern)
Supervisor:
Niedermayer, Christof (Ekstern)
Vegge, Tejs (Intern)
Main Supervisor:
Christensen, Niels Bech (Intern)
Examiner:
Schiøtz, Jakob (Intern)
Lake, Alysia Catherine Isabel (Ekstern)
Luetkens, Hubertus (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut, samfinansiering
Project: PhD
Methanol Synthesis for Sustainable Fuel Synthesis

Department of Physics
Period: 15/03/2010 → 17/06/2013
Number of participants: 6
Phd Student:
Sharafutdinov, Irek (Intern)
Supervisor:
Nielsen, Jane Hvolbæk (Intern)
Main Supervisor:
Chorkendorff, Ib (Intern)
Examiner:
Chakraborty, Debasish (Intern)
Armbrüster, Marc (Ekstern)
Sehested, Jens (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Quantum Information Processing with Schrödinger Cat States

Department of Physics
Period: 15/03/2010 → 30/08/2013
Number of participants: 5
Phd Student:
Laghaout, Amine (Intern)
Main Supervisor:
Andersen, Ulrik Lund (Intern)
Examiner:
Brusch, Anders (Ekstern)
Bourennane, Mohamed (Ekstern)
Marquardt, Christoph Dirk (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Catalytic conversion of carbohydrates

Department of Physics
Period: 01/03/2010 → 19/04/2013
Number of participants: 6
Phd Student:
Osmundsen, Christian Mårup (Intern)
Supervisor:
Taarning, Esben (Intern)
Main Supervisor:
Rossmeisl, Jan (Intern)
Examiner:
Fristrup, Peter (Intern)
Skrydstrup, Troels (Ekstern)
Svelle, Stian (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD
Real-time radiation dosimetry for improved patient safety in brachy therapy

Department of Physics
Period: 01/03/2010 → 26/02/2014
Number of participants: 6
Phd Student:
Kertzscher Schwencke, Gustavo Adolfo Vladimir (Intern)
Supervisor:
Tanderup, Kari (Ekstern)
Main Supervisor:
Andersen, Claus E. (Ekstern)
Examiner:
Lauritzen, Bent (Intern)
Baltas, Dimos (Ekstern)
Tedgren, Åsa Karin Carlsson (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Programbevilling
Project: PhD

Monte Carlo based treatment plans for radiotherapy

Department of Physics
Period: 01/02/2010 → 30/09/2012
Number of participants: 7
Phd Student:
Cronholm, Rickard (Intern)
Supervisor:
Behrens, Claus F. (Ekstern)
Helt-Hansen, Jakob (Intern)
Main Supervisor:
Andersen, Claus E. (Ekstern)
Examiner:
Jensen, Mikael (Intern)
Chakarova, Roumiana (Ekstern)
Malinen, Eirik (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Band Gap Design and Light Harvesting

Department of Physics
Period: 01/01/2010 → 22/03/2013
Number of participants: 7
Phd Student:
Cavalca, Filippo Carlo (Intern)
Supervisor:
Damsgaard, Christian Danvad (Intern)
Wagner, Jakob Birkedal (Intern)
Main Supervisor:
Hansen, Thomas Willum (Intern)
Examiner:
Melhave, Kristian (Intern)
Gamez, José Juan Calvino (Ekstern)
Zaluzec, Nestor J. (Ekstern)
Catalysts for synthesis of methanol and higher alcohols from syngas

Department of Physics
Period: 01/01/2010 → 19/04/2013
Number of participants: 7
Phd Student:
Duchstein, Linus Daniel Leonhard (Intern)
Supervisor:
Damsgaard, Christian Danvad (Intern)
Hansen, Thomas Willum (Intern)
Main Supervisor:
Wagner, Jakob Birkedal (Intern)
Examiner:
Horch, Sebastian (Intern)
Datye, Abhaya K. (Ekstern)
Willinger, Marc-Georg (Ekstern)

A surface science approach for finding new materials for photo catalysis

Department of Physics
Period: 01/11/2009 → 07/03/2013
Number of participants: 6
Phd Student:
Dionigi, Fabio (Intern)
Supervisor:
Vesborg, Peter Christian Kjærgaard (Intern)
Main Supervisor:
Chorkendorff, Ib (Intern)
Examiner:
Nielsen, Jane Hvolbæk (Intern)
Chakarov, Dinko (Ekstern)
van de Krol, Roel (Ekstern)

Optical quantum feedback systems for applications in biosensing and quantum information processing

Department of Physics
Period: 01/11/2009 → 30/04/2012
Number of participants: 5
Phd Student:
Usuga Castaneda, Mario A. (Intern)
Main Supervisor:
Andersen, Ulrik Lund (Intern)
Examiner:
Hansen, Jern Otto Bindslev (Ekstern)
Korolkova, Natalia (Ekstern)
Thomsen, Jan Westenkær (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: 1/3 DTU-stip, 2/3 FUR/andet
Project: PhD

**Time dependent density functional theory applied to molecular electronics**
Department of Physics
Period: 01/10/2009 → 28/02/2013
Number of participants: 3
Phd Student:
Glinsvad, Christian (Intern)
Supervisor:
Thygesen, Kristian Sommer (Intern)
Main Supervisor:
Schiøtz, Jakob (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

**Design of materials for photo catalytic splitting of water**
Department of Physics
Period: 01/09/2009 → 28/09/2012
Number of participants: 6
Phd Student:
Laursen, Anders Bo (Intern)
Supervisor:
Vesborg, Peter Christian Kjærgaard (Intern)
Main Supervisor:
Chorkendorff, Ib (Intern)
Examiner:
Schiøtz, Jakob (Intern)
Nielsen, Michael Brorson (Intern)
Hu, Xile (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Globaliseringsmidler
Project: PhD

**Struktur og reaktivitet af nanopartikler med betydning for katalytiske processer**
Department of Physics
Period: 01/09/2009 → 22/03/2013
Number of participants: 6
Phd Student:
Strebel, Christian Ejersbo (Intern)
Supervisor:
Nielsen, Jane Hvolbæk (Intern)
Main Supervisor:
Chorkendorff, Ib (Intern)
Examiner:
Nielsen, Martin Meedom (Intern)
Sehested, Jens (Intern)
de Jongh, Petra E. (Ekstern)
Design of zeolite catalysts for selective benzene to cyclohexene hydrogenation

Department of Physics
Period: 01/08/2009 → 21/09/2012
Number of participants: 6
Phd Student:
Wellendorff, Jess (Intern)
Supervisor:
Bligaard, Thomas (Intern)
Main Supervisor:
Jacobsen, Karsten Wedel (Intern)
Examiner:
Rossmeisl, Jan (Intern)
Hellman, Anders (Ekstern)
Michaelides, Angelos (Ekstern)

Inclusion of dispersion effects in density functional theory: Development and application

Department of Physics
Period: 01/07/2009 → 22/08/2012
Number of participants: 6
Phd Student:
Møgelhøj, Andreas (Intern)
Supervisor:
Nørskov, Jens Kehlet (Intern)
Main Supervisor:
Jacobsen, Karsten Wedel (Intern)
Examiner:
Brandbyge, Mads (Intern)
Jónsson, Hannes (Ekstern)
Mikkelsen, Kurt V. (Ekstern)

Advanced Characterization of One-dimensional Nanowires for Photovoltaics by Electron Microscopy

Department of Physics
Period: 01/05/2009 → 19/12/2012
Number of participants: 6
Phd Student:
Persson, Johan Mikael (Intern)
Supervisor:
Dunin-Borkowski, Rafał E. (Intern)
Main Supervisor:
Wagner, Jakob Birkedal (Intern)
Examiner:
Yvind, Kresten (Intern)
Helvoort, Antonius T. J. van (Ekstern)
Johnson, Erik (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Anden EU-finansiering
Project: PhD

**Quantum information processing with mesoscopic photonic states**
Department of Physics
Period: 01/05/2009 → 25/10/2012
Number of participants: 5
Phd Student:
Madsen, Lars Skovgaard (Intern)
Main Supervisor:
Andersen, Ulrik Lund (Intern)
Examiner:
Hald, Jan (Ekstern)
Paris, Matteo G. A. (Ekstern)
Schnabel, Roman (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Anden EU-finansiering
Project: PhD

**Strong nonlinear effects in a diamond-plasmon system**
Department of Physics
Period: 01/02/2009 → 28/09/2012
Number of participants: 5
Phd Student:
Kumar, Shailesh (Intern)
Main Supervisor:
Andersen, Ulrik Lund (Intern)
Examiner:
Wubs, Martijn (Intern)
Benson, Oliver (Ekstern)
Lodahl, Peter (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Eksternt finansieret virksomhed
Project: PhD

**Generation of Optical Shrödinger Cat-States**
Department of Physics
Period: 01/01/2009 → 21/06/2012
Number of participants: 6
Phd Student:
Tipsmark, Anders (Intern)
Supervisor:
Tidemand-Lichtenberg, Peter (Intern)
Main Supervisor:
Andersen, Ulrik Lund (Intern)
Examiner:
Rottwitt, Karsten (Intern)
Chekhova, Maria V. (Ekstern)
Filip, Radim (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

In-situ TEM observation of growth and properties of group-IV doped and SiGe heterostructure nanowires

Department of Physics
Period: 01/01/2009 → 30/04/2012
Number of participants: 8
Phd Student:
Pennington, Robert Scott (Intern)
Supervisor:
Boothroyd, Chris (Intern)
Dunin-Borkowski, Rafał E. (Intern)
Wagner, Jakob Birkedal (Intern)
Main Supervisor:
Hansen, Jørn Otto Bindslev (Ekstern)
Examiner:
Thygesen, Kristian Sommer (Intern)
Rosenauer, Andreas (Ekstern)
Rouviere, Jean-Luc (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut/centerfinansieret
Project: PhD

Water Splitting Reaction at Semiconductor Surfaces

Department of Physics
Period: 01/01/2009 → 23/02/2012
Number of participants: 7
Phd Student:
Zawadzki, Paweł (Intern)
Supervisor:
Jacobsen, Karsten Wedel (Intern)
Rossmeisl, Jan (Intern)
Main Supervisor:
Nørskov, Jens Kehlet (Intern)
Examiner:
Chorkendorff, Ib (Intern)
Jónsson, Hannes (Ekstern)
Marzari, Nicola (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Udvikling og design af et mikrobølgemodtagersystem til måling af hurtige ioner i fusionseksperimenter

Department of Physics
Period: 15/12/2008 → 29/05/2012
Number of participants: 7
Phd Student:
Furtula, Vedran (Intern)
Supervisor:
Fast Ion Dynamics in ASDEX Upgrade Measured by Collective Thomson Scattering

Department of Physics
Period: 01/11/2008 → 29/03/2012
Number of participants: 6
Phd Student:
Moseev, Dmitry (Intern)
Supervisor:
Meo, Fernando (Intern)
Main Supervisor:
Korsholm, Søren Bang (Intern)
Examiner:
Bohr, Tomas (Intern)
Ericsson, Göran (Ekstern)
García-Munoz, Manuel (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut/centerfinansieret
Project: PhD

Development of e-learning courses in environmental technology and physics.
With Moodle as platform 4 e-learning courses in environmental technology and physics is developed. The 4 courses are:

Department of Environmental Engineering

Department of Physics
Period: 01/09/2008 → 30/06/2011
Number of participants: 5
Acronym: IKT-støttet læring
Project ID: 30626
Project participant:
Arvin, Erik (Intern)
Mikkelsen, Peter Steen (Intern)
Rasmussen, Birte Kastrup (Intern)
Knudsen, Carsten (Intern)
Project Manager, organisational:
Eriksson, Eva (Intern)

Financing sources
Source: Uddannelse. Statslige. Andre statslige
Name of research programme: Ukendt
Amount: 900,000.00 Danish Kroner
Project
Electron Transport and Chemistry of Graphene

Department of Physics
Period: 01/09/2008 → 30/09/2011
Number of participants: 6
Phd Student: Vanin, Marco (Intern)
Supervisor: Jacobsen, Karsten Wedel (Intern)
Main Supervisor: Thygesen, Kristian Sommer (Intern)
Examiner: Brandbyge, Mads (Intern)
Brocks, Geert H. L. A. (Ekstern)
Hornekær, Liv (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Katalytiske og elektroniske egenskaber af metalnanopartikler

Department of Physics
Period: 01/09/2008 → 20/01/2012
Number of participants: 6
Phd Student: Larsen, Ask Hjorth (Intern)
Supervisor: Thygesen, Kristian Sommer (Intern)
Main Supervisor: Jacobsen, Karsten Wedel (Intern)
Examiner: Rossmeisl, Jan (Intern)
Grönbeck, Henrik (Ekstern)
Manninen, Matti Jussi (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.
Project: PhD

New nanomaterials for oxygen evolution electrodes

Department of Physics
Period: 01/09/2008 → 29/05/2012
Number of participants: 6
Phd Student: Johansson, Tobias Peter (Intern)
Supervisor: Nielsen, Jane Hvolbæk (Intern)
Main Supervisor: Chorkendorff, Ib (Intern)
Examiner: Frandsen, Cathrine (Intern)
Arenz, Matthias (Ekstern)
Nilsson, Anders (Ekstern)

Financing sources
Singularities in fluid flows

Department of Physics
Period: 01/09/2008 → 21/06/2012
Number of participants: 6
Phd Student:
Tophøj, Laust Emil Hjerrild (Intern)
Supervisor:
Aref, Hassan (Intern)
Main Supervisor:
Bohr, Tomas (Intern)
Examiner:
Rasmussen, Jens Juul (Intern)
Eckhardt, Bruno (Ekstern)
Fabre, David (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Site selectivity of specific reaction steps important for catalysis

Department of Physics
Period: 01/09/2008 → 21/12/2011
Number of participants: 5
Phd Student:
Nielsen, Kenneth (Intern)
Main Supervisor:
Nielsen, Jane Hvolbæk (Intern)
Examiner:
Dahl, Søren (Ekstern)
Diekhöner, Lars (Ekstern)
Juurlink, Ludo (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Forøgelse af kemisk aktivitet ved brug af varme elektroner

Department of Physics
Period: 01/08/2008 → 22/03/2013
Number of participants: 6
Phd Student:
Jensen, Robert Steen Raunsgaard (Intern)
Supervisor:
Hansen, Ole (Intern)
Main Supervisor:
Chorkendorff, Ib (Intern)
Examiner:
Vegge, Tejs (Intern)
Jaramillo, Thomas Francisco (Ekstern)
Quaade, Ulrich (Intern)

Financing sources
**Strongly coupled diamond-plasmon system using nanowires**

Department of Physics  
Period: 01/08/2008 → 01/03/2010  
Number of participants: 4  
Phd Student:  
Shakoor, Abdul (Intern)  
Supervisor:  
Hansen, Jørn Otto Bindslev (Ekstern)  
Lodahl, Peter (Intern)  
Main Supervisor:  
Andersen, Ulrik Lund (Intern)

**Financing sources**

Source: Internal funding (public)  
Name of research programme: Grundforskningsfonden  
Project: PhD

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**Funktionelle superledende og magnetiske materialer til energianvendelser**

Department of Physics  
Period: 01/07/2008 → 29/03/2012  
Number of participants: 6  
Phd Student:  
Toft-Petersen, Rasmus (Intern)  
Supervisor:  
Abrahamsen, Asger Bech (Intern)  
Main Supervisor:  
Andersen, Niels Hessel (Intern)  
Examiner:  
Jacobsen, Claus Schelde (Intern)  
Eskildsen, Morten Ring (Intern)  
McEwen, Keith Alistair (Ekstern)

**Financing sources**

Source: Internal funding (public)  
Name of research programme: Eksternt finansieret virksomhed  
Project: PhD

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**Materials Informatics**

Department of Physics  
Period: 01/06/2008 → 30/04/2012  
Number of participants: 6  
Phd Student:  
Landis, David Dominic (Intern)  
Supervisor:  
Bligaard, Thomas (Intern)  
Main Supervisor:  
Jacobsen, Karsten Wedel (Intern)  
Examiner:  
Schiatz, Jakob (Intern)  
Enkovaara, Jussi (Ekstern)  
Moses, Poul Georg (Intern)

**Financing sources**

Source: Internal funding (public)
Name of research programme: **Offentlig finansiering**
Project: PhD

**Supporting and stabilizing biomimetic membranes**
Department of Physics  
Period: 01/06/2008 → 28/09/2011  
Number of participants: 6  
Phd Student: Ibragimova, Sania (Intern)  
Supervisor: Hélix-Nielsen, Claus (Intern)  
Main Supervisor: Bohr, Henrik (Intern)  
Examiner: Berg-Sørensen, Kirstine (Intern)  
Höök, Fredrik (Ekstern)  
Klösgen, Beate (Ekstern)

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: DTU-lønnet stipendie  
Project: PhD

**Theoretical study of cathode Materials in Direct Methanol and Proton exchange Membrane fuel cell**
Department of Physics  
Period: 01/03/2008 → 20/04/2011  
Number of participants: 6  
Phd Student: Tritsaris, Georgios (Intern)  
Supervisor: Nørskov, Jens Kehlet (Intern)  
Main Supervisor: Rossmeisl, Jan (Intern)  
Examiner: Dahl, Søren (Ekstern)  
Arenz, Matthias (Ekstern)  
Eikerling, Michael H. (Ekstern)

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: DTU-lønnet stipendie  
Project: PhD

**Theoretical study of Photo-Catalytic oxygen evolution**
Department of Physics  
Period: 01/03/2008 → 01/06/2011  
Number of participants: 5  
Phd Student: Man, Isabela Costinela (Intern)  
Main Supervisor: Rossmeisl, Jan (Intern)  
Examiner: Thygesen, Kristian Sommer (Intern)  
Hellman, Anders (Ekstern)  
Krtíl, Petr (Ekstern)

**Financing sources**  
Source: Internal funding (public)
**Accurate treatment of nanoelectronics through improved description of van der Waals Interactions**

Department of Physics  
Period: 01/02/2008 → 20/04/2011  
Number of participants: 7  
Phd Student: Kelkkanen, Kari André (Intern)  
Supervisor: Lundqvist, Bengt I. (Ekstern)  
Nørskov, Jens Kehlet (Intern)  
Main Supervisor: Jacobsen, Karsten Wedel (Intern)  
Examiner: Rossmeis, Jan (Intern)  
Mahan, Gerald Dennis (Ekstern)  
Michaelides, Angelos (Ekstern)  

**Financing sources**  
Source: Internal funding (public)

**Ædelmetalkatalysatore til rensning af røg fra dieselmotorer**

Department of Physics  
Period: 01/02/2008 → 28/09/2011  
Number of participants: 7  
Phd Student: Simonsen, Søren Bredmose (Intern)  
Supervisor: Dahl, Søren (Intern)  
Helveg, Stig (Ekstern)  
Main Supervisor: Chorkendorff, Ib (Intern)  
Examiner: Hansen, Thomas Willum (Intern)  
Crozier, Peter A. (Ekstern)  
Olsson, Eva (Ekstern)  

**Financing sources**  
Source: Internal funding (public)

**Fluctuations and phase transitions in quenched superconducting rings and annular Josephson junctions**

Department of Physics  
Period: 01/02/2008 → 30/11/2011  
Number of participants: 8  
Phd Student: Gordeeva, Anna Valekjevna (Intern)  
Supervisor: Mygind, Jesper (Intern)  
Pankratov, Andrey (Ekstern)  
Sørensen, Mads Peter (Intern)  
Main Supervisor: Jacobsen, Claus Schelde (Intern)
Examiner:
Hansen, Jørn Otto Bindslev (Ekstern)
Kuzmin, Leonid (Ekstern)
Nygård, Jesper (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

**Efficient Catalysts for PEM Fuel Cells**
Department of Physics
Period: 15/01/2008 → 21/06/2012
Number of participants: 6
Phd Student:
Shim, Signe Sarah (Intern)
Supervisor:
Andersen, Steen Yde (Ekstern)
Main Supervisor:
Chorkendorff, Ib (Intern)
Examiner:
Nielsen, Jane Hvolbæk (Intern)
Herbst, Konrad (Ekstern)
Hjuler, Hans Aage (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: ErhvervsPhD-ordningen VTU
Project: PhD

**Biological Oxygen Reduction Reaction**
Department of Physics
Period: 01/01/2008 → 30/05/2008
Number of participants: 3
Phd Student:
Kjærgaard, Christian Hauge (Intern)
Supervisor:
Rossmeisl, Jan (Intern)
Main Supervisor:
Nørskov, Jens Kehlet (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

**size dependent reactivity of metal clusters**
Department of Physics
Period: 01/01/2008 → 24/08/2012
Number of participants: 5
Phd Student:
Fiordaliso, Elisabetta Maria (Intern)
Main Supervisor:
Chorkendorff, Ib (Intern)
Examiner:
Horch, Sebastian (Intern)
Törnqvist, Eric (Ekstern)
Züttel, Andreas (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

**Bifucational and translational studies of nephron autoregulation**
Department of Physics
Period: 01/12/2007 → 02/03/2011
Number of participants: 6
Phd Student:
Laugesen, Jakob Lund (Intern)
Supervisor:
Sosnovtseva, Olga (Intern)
Main Supervisor:
Mosekilde, Erik (Intern)
Examiner:
Serensen, Mads Peter (Intern)
Colding-Jørgensen, Morten (Ekstern)
Postnov, Dmitry (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Anden EU-finansiering
Project: PhD

**Materials for Superconducting wind turbine generators**
Department of Physics
Period: 15/11/2007 → 19/04/2013
Number of participants: 6
Phd Student:
Khoryushin, Alexey (Intern)
Supervisor:
Jacobsen, Claus Schelde (Intern)
Mozhaev, Peter (Intern)
Main Supervisor:
Hansen, Jørn Otto Bindslev (Ekstern)
Examiner:
Lukichev, Vladimir F. (Ekstern)
Paturi, Petriina (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Globaliseringsmidler
Project: PhD

**Inexpensive Electrocatalysts for O2 Reduction**
Department of Physics
Period: 01/11/2007 → 02/02/2011
Number of participants: 6
Phd Student:
Vallejo, Federico Calle (Intern)
Supervisor:
Nørskov, Jens Kehlet (Intern)
Main Supervisor:
Rossmeisl, Jan (Intern)
Ultra rene elektroder og elektrolytter for SOFC (Ultra Clean electrode and electrolytes for SOFC)

Department of Physics
Period: 01/11/2007 → 22/06/2011
Number of participants: 7
Phd Student:
Andersen, Thomas (Intern)
Supervisor:
Hansen, Karin Vels (Intern)
Mogensen, Mogens Bjerg (Intern)
Main Supervisor:
Chorkendorff, Ib (Intern)
Examiner:
Rossmeisl, Jan (Intern)
Irvine, John T. S. (Ekstern)
Morgen, Per (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Programbevilling
Project: PhD

Direct NO decomposition over non-transition metal surfaces

Department of Physics
Period: 01/10/2007 → 20/04/2011
Number of participants: 5
Phd Student:
Jiang, Tao (Intern)
Main Supervisor:
Bligaard, Thomas (Intern)
Examiner:
Thygesen, Kristian Sommer (Intern)
Lopez, Nuria (Intern)
Jónsson, Hannes (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Quantum Mechanical Calculations on Metalloproteins

Department of Physics
Number of participants: 5
Phd Student:
Greisen, Per Junior (Intern)
Main Supervisor:
Bohr, Henrik (Intern)
Fluid Dynamics of Animal Locomotion

Department of Physics
Period: 15/08/2007 → 02/02/2011
Number of participants: 8
Phd Student:
Schnipper, Teis (Intern)
Supervisor:
Aref, Hassan (Intern)
Bohr, Tomas (Intern)
Sørensen, Jens Nørkær (Intern)
Main Supervisor:
Andersen, Anders Peter (Intern)
Examiner:
Brøns, Morten (Intern)
Water, Willem van de (Ekstern)
Williamson, Charles H. K. (Ekstern)

Resonance-Assisted Hot-Electron Femtochemistry at Surfaces

Department of Physics
Period: 01/08/2007 → 08/12/2010
Number of participants: 5
Phd Student:
Olsen, Thomas (Intern)
Main Supervisor:
Schiøtz, Jakob (Intern)
Examiner:
Vegge, Tejs (Intern)
Reuter, Karsten (Ekstern)
Voorhis, Troy Van (Ekstern)

Theoretical study of the oxygen reduction reaction

Department of Physics
Period: 01/08/2007 → 08/12/2010
Number of participants: 6
Phd Student:
Tripkovic, Vladimir (Intern)
Supervisor:
Mechanism-Based Modeling of Cellular Interactions: From Physics to Systems Biology

Biophysics and Fluids

Department of Physics
Period: 01/04/2007 → 31/03/2010
Number of participants: 1
Project Manager, organisational:
Sosnovtseva, Olga (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-lønnet stipendie
Project: PhD

Theoretical study of ammonia synthesis under ambient conditions

Department of Physics
Period: 01/04/2007 → 02/03/2011
Number of participants: 7
PhD Student:
Petzold, Vivien Gabriele (Intern)
Supervisor:
Bligaard, Thomas (Intern)
Nørskov, Jens Kehlet (Intern)
Main Supervisor:
Jacobsen, Karsten Wedel (Intern)
Examiner:
Thygesen, Kristian Sommer (Intern)
Hyldgaard, Per (Ekstern)
Reuter, Karsten (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-lønnet stipendie
Project: PhD

Size and structure dependent reactivity of nanoparticles

Department of Physics
Period: 01/03/2007 → 29/09/2010
Number of participants: 6
PhD Student:
Olsen, Jakob Lind (Intern)
Supervisor:
Hansen, Ole (Intern)
Main Supervisor:
Generation and Characterisation of Non-Classical Surface Plasmons

Department of Physics
Period: 01/02/2007 → 31/03/2010
Number of participants: 7
PhD Student:
Huck, Alexander (Intern)
Supervisor:
Lodahl, Peter (Intern)
Sørensen, Anders S (Ekstern)
Main Supervisor:
Andersen, Ulrik Lund (Intern)
Examiner:
Kneipp, Katrin (Intern)
Bozhevolnyi, Sergey I. (Intern)
Jelezko, Fedor (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-lønnet stipendie
Project: PhD

Teoretiske studier af Fischer-Tropsch reaktionen

Department of Physics
Period: 01/01/2007 → 30/04/2012
Number of participants: 6
PhD Student:
Toftelund, Anja (Intern)
Supervisor:
Bligaard, Thomas (Intern)
Main Supervisor:
Rossmeisl, Jan (Intern)
Examiner:
Vegge, Tejs (Intern)
Lopez, Nuria (Intern)
Hellman, Anders (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 DTU-stip, 2/3 FUR/andet
Project: PhD

Udforskning af nye nano strukturerede materialer til fremstilling af hydrogen

Department of Physics
Period: 15/10/2006 → 21/04/2010
Number of participants: 5
PhD Student:
Multiscale Neuron-glial communications

Department of Physics
Period: 01/10/2006 → 21/04/2010
Number of participants: 5
PhD Student:
Faurby-Bentzen, Christian Krefeld (Intern)
Main Supervisor:
Mosekilde, Erik (Intern)
Examiner:
Berg-Sørensen, Kirstine (Intern)
Braun, Hans Albert (Ekstern)
Jensen, Kimmo (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-lønnet stipendie
Project: PhD

European Network of Funding Agencies - Coordination of National Complexity Research and Training Activities : EU contract no 036195

Complexity and complex systems is an emergent and rapidly growing research field with a large technological potential, in which Europe has fostered scientific excellence with extensive collaboration across Europe and abroad. Based on the need to put stronger focus on this field and to further its high growth potential, 11 European Research Councils and Ministries initiated a consortium, in the form of a specific support action, aiming to establish the necessary environment for coordinating nationally strategically planned research activities.
Multiscale intercellular communications: From experiment to mechanism-based modeling

The proposal offers an approach to studying intercellular communications that combines innovative techniques from Biophysics and Physiology with newly developed methods and concepts from Systems Biology and Complex Systems Theory. We propose a research project that integrates experimental investigations of cell-to-cell signaling in neuronal systems at different time and length scales with nonlinear time-series analysis and mechanism-based modeling of pathways, interactions and rhythmic patterns. We believe that this approach can provide new understanding of the functioning of the central nervous system under normal and pathological conditions. Such understanding is obviously essential for a better treatment of patients with mental disorders. The project is based on a unique interdisciplinary collaboration and serves to stimulate the use of biosimulation in Denmark.

Simulering af dynamiske fænomener i bloodflowregulering

Department of Mathematics
Period: 01/09/2006 → 31/08/2009
Number of participants: 6
Acronym: Complexity-NET
Project participant:
Sørensen, Mads Peter (Intern)
Mosekilde, Erik (Intern)
Jensen, Mogens Hegh (Ekstern)
Sørensen, Preben Graae (Ekstern)
Sibani, Paolo (Ekstern)
Project Manager, organisational:
Alstrøm, Preben (Ekstern)

Financing sources
Source: Forsk. EU - Andre EU-midler
Name of research programme: Forsk. EU - Andre EU-midler
Amount: 1,900,000.00 Danish Kroner

Biophysics and Fluids

Department of Physics
Period: 01/09/2006 → 02/06/2010
Number of participants: 5
Phd Student:
Larsen, Peter (Intern)
Main Supervisor:
Mosekilde, Erik (Intern)
Examiner:
Sørensen, Mads Peter (Intern)
Bie, Peter (Ekstern)
Thomas, Stephen Randall (Ekstern)
Desity Functional Theory Studies of Oxides in Catalysis

Department of Physics
Number of participants: 6
Phd Student:
Hansen, Heine Anton (Intern)
Supervisor:
Rossmeisl, Jan (Intern)
Main Supervisor:
Nørskov, Jens Kehlet (Intern)
Examiner:
Schiøtz, Jakob (Intern)
Alonso, Núria López (Ekstern)
Koper, Marcus Theodorus Maria (Ekstern)

Elektrontransport i Nanostrukturer

Department of Physics
Period: 15/08/2006 → 10/02/2010
Number of participants: 6
Phd Student:
Rostgaard, Carsten (Intern)
Supervisor:
Thygesen, Kristian Sommer (Intern)
Main Supervisor:
Jacobsen, Karsten Wedel (Intern)
Examiner:
Bligaard, Thomas (Intern)
Gao, Shiwu (Ekstern)
van Leeuwen, Robert (Ekstern)

Simuleringer af styrende mekanismer for initiering af metal dusting korrosion

Department of Physics
Period: 15/08/2006 → 17/02/2010
Number of participants: 8
Phd Student:
Saadi, Souheil (Intern)
Supervisor:
Appel, Charlotte Clausen (Intern)
Helveg, Stig (Ekstern)
Hinnemann, Berit (Intern)
Main Supervisor:
Nørskov, Jens Kehlet (Intern)
Næste generation af steam reforming katalysatorer

Department of Physics
Period: 01/08/2006 → 22/09/2010
Number of participants: 7
Phd Student: Jakobsen, Jon Geest (Intern)
Supervisor: Sehested, Jens (Intern)
Sørensen, Esben Lauge (Ekstern)
Main Supervisor: Chorkendorff, Ib (Intern)
Examiner: Nielsen, Jane Hvolbæk (Intern)
Chen, De (Ekstern)
Hensen, Emiel J. M. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: ErhvervsPhD-ordningen VTU
Project: PhD

A new way to test beta cell functionality in health and diabetes

Department of Physics
Period: 01/07/2006 → 30/11/2011
Number of participants: 6
Phd Student: Korsgaard, Thomas Vagn (Intern)
Supervisor: Colding-Jørgensen, Morten (Ekstern)
Main Supervisor: Mosekilde, Erik (Intern)
Examiner: Berg-Sørensen, Kirstine (Intern)
Madsbad, Sten (Ekstern)
Westerhoff, Hans V. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: ErhvervsPhD-ordningen VTU
Project: PhD

Magnetism and Superconducting Annuli

Department of Physics
Period: 01/04/2006 → 27/05/2009
Number of participants: 6
Phd Student: Aarøe, Morten (Intern)
Supervisor:
Bøggild, Peter (Intern)
Main Supervisor:
Mygind, Jesper (Intern)
Examiner:
Jacobsen, Claus Schelde (Intern)
Arutyunov, Konstantin (Ekstern)
Ustinov, Alexey V. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-lønnet stipendie
Project: PhD

Analyse af nanopartiklers funktionalitet og betydningen af den enkelte partikels morfologi
Department of Physics
Period: 01/03/2006 → 04/11/2009
Number of participants: 6
Phd Student:
Nielsen, Rasmus Munksgård (Intern)
Supervisor:
Johansson, Martin (Intern)
Main Supervisor:
Chorkendorff, Ib (Intern)
Examiner:
Hansen, Ole (Intern)
Palmér, Richard E. (Ekstern)
Sehested, Jens (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-lønnet stipendie
Project: PhD

Composite Fibre and Solid-State Visible Light Source
Department of Physics
Period: 01/03/2006 → 23/09/2009
Number of participants: 6
Phd Student:
Andersen, Martin Thalbitzer (Intern)
Supervisor:
Pedersen, Christian (Intern)
Main Supervisor:
Tidemand-Lichtenberg, Peter (Intern)
Examiner:
Petersen, Paul Michael (Intern)
Arie, Ady (Ekstern)
Dunn, Malcolm (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU, Samfinansiering
Project: PhD

HEFatS - En tunnelediode elektronemitter tilgang
Department of Physics
Period: 01/03/2006 → 27/05/2009
Number of participants: 6
Phd Student:
Thomsen, Lasse Bjørchmar (Intern)
Supervisor:
Hansen, Ole (Intern)
Main Supervisor:
Chorkendorff, Ib (Intern)
Examiner:
Schietz, Jakob (Intern)
Chakarov, Dinko (Ekstern)
Diesing, Detlef (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Grundforskningsfonden
Project: PhD

Modelling the Shape and Reactivity of Metallic Nanoparticles
Department of Physics
Period: 01/02/2006 → 05/05/2009
Number of participants: 5
Phd Student:
Gavnholt, Jeppe (Intern)
Main Supervisor:
Schietz, Jakob (Intern)
Examiner:
Jacobsen, Karsten Wedel (Intern)
Hyldgaard, Per (Ekstern)
Häkkinen, Hannu (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-lønnet stipendie
Project: PhD

Tæthedsfunktional teori (DFT) simuleringer af metan omdannelse i enzymer og i uorganiske katalysatorer
Department of Physics
Period: 01/02/2006 → 05/05/2009
Number of participants: 6
Phd Student:
Hummelshøj, Jens Strabo (Intern)
Supervisor:
Vegge, Tejs (Intern)
Main Supervisor:
Nørskov, Jens Kehlet (Intern)
Examiner:
Nielsen, Jane Hvolbæk (Intern)
Wolverton, Chris M. (Ekstern)
Züttel, Andreas (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Anden EU-finansiering
Project: PhD

The Balance between Glucose and Lipid Metabolism in Lean, Obese and Diabetic Persons. A Biosimulation Approach
Department of Physics
Period: 01/02/2006 → 21/04/2010
Number of participants: 6
Phd Student:
Hallgreen, Christine E. (Ekstern)

Supervisor:
Colding-Jørgensen, Morten (Ekstern)

Main Supervisor:
Mosekilde, Erik (Intern)
Examiner:
Knudsen, Carsten (Intern)
Miles, John M. (Ekstern)
Thirstrup, Steffen (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: ErhvervsPhD-ordningen VTU
Project: PhD

Norvel Efficient Solid Storage for Hydrogen (Nesshy)
Department of Physics
Risø National Laboratory for Sustainable Energy
Center for Nanoteknologi
National Centre for Scientific Research "Demokritos"
University of Salford
AIR LIQUIDE
European Commission - Joint Research Center
Stockholm University
Institutt for Energiteknikk
University of Fribourg
University of Birmingham
Vrije Universiteit Amsterdam
Centre National de la Recherche Scientifique
DaimlerChrysler AG
GKSS Forschungszentrum Geesthacht GmbH
University of Iceland
Johnson Matthey Plc
Forschungs Zentrum Karlsruhe GmbH
Max Planck Institute
Middle East Technical University
Instituto Nacional de Engenharia, Tecnologia e Inovacao
Leibniz-Institut für Festkörper- und Werkstoffforschung Dresden e.V
Delft University of Technology
Southwest Research Institute
Period: 01/01/2006 → 31/12/2010
Number of participants: 2
Project ID: 20244
Project participant:
Vegge, Tejs (Ekstern)
Phase stability of interstitial austenitic steel
The project is a combined experimental and theoretical approach to establish the basic thermodynamic data for ternary austenitic FeCrNi with a view to improve the stability of steels hardened by insertion of interstitial nitrogen and/or carbon.

Physics of Living Cells
Department of Physics
Period: 01/01/2006 → 31/12/2008
Number of participants: 1
Project Manager, organisational: Moskilde, Erik (Intern)

Computational Atomic-scale Materials Physics
Installation and operation of a Linux cluster
Department of Physics
Center for Nanoteknologi
Period: 22/12/2005 → 31/12/2008
Number of participants: 1
Project Manager, organisational: Jacobsen, Karsten Wedel (Intern)

Financing sources
Source: Forskningsprojekter - Andre ministerier og styrelser
Name of research programme: Forskningsprojekter - Andre ministerier og styrelser
Amount: 3,500,000.00 Danish Kroner
Project
Towards 25% efficiency solar cells: additional funding

Department of Physics
Center for Individual Nanoparticle Functionality
Center for Nanoteknologi
Topsil Semiconductor Materials A/S
Period: 05/12/2005 → 15/09/2006
Number of participants: 1
Project ID: 20233
Project Manager, organisational:
Schiøtz, Jakob (Intern)

Financing sources
Source: Forskningsrådene - Andre
Name of research programme: Forskningsrådene - Andre
Amount: 347,200.00 Danish Kroner

Development of an Integrated MEMS (Micro Electro Mechanical System) based on DNA Analysis

Department of Micro- and Nanotechnology
BioLabChip
Department of Physics
Biophysics and Fluids
D'Appolonia S.p.A.
Delft University of Technology
Institut für Mikrotechnik Mainz GmbH
Uppsala University Hospital
Period: 01/12/2005 → 31/05/2009
Number of participants: 3
Acronym: SMART-BioMEMS
Project ID: IST-016554
Number of related Ph.D. students: 1
Project participant:
Wolff, Anders (Intern)
Brivo, Monica (Intern)
Bruus, Henrik (Intern)

Relations
Publications:
A simple and efficient method for on-chip storage of reagents: towards lab-on-a-chip systems for point-of-care DNA diagnostics
On-Chip integration of sample pretreatment and Multiplex polymerase chain reaction (PCR) for DNA analysis
Dried reagents for multiplex genotyping by tag-array minisequencing to be used in microfluidic devices
A simple and efficient method for reducing surface roughness of polymer microstructure
Ultrasonic mixing in polymer microfluidics
On-Chip Integration of Sample Pretreatment and Multiplex Polymerase Chain Reaction (PCR) for DNA Analysis
Development of a lab-on-a-chip device for point-of-care genetic diagnostics
A Total Integrated Biochip System for Detection of SNP in Cancer

Otto Mønsted guest professorship
Department of Physics
Stability of Magnetic Nanoparticles in Magnetic Beads

The chemical stability of magnetic particles is of great importance for their applications in medicine and biotechnology. By use of Mössbauer spectroscopy and magnetization measurements, we study the kinetics of transformation of nanoparticles of magnetite to maghemite during exposure to air under ambient conditions and during exposure to different chemical treatments.

Department of Physics

Department of Micro- and Nanotechnology

Technische Universität Clausthal

Period: 01/09/2005 → 30/06/2006

Number of participants: 4

Project ID: 20212

Project participant:

Chen, Wei (Intern)

Hansen, Mikkel Fougt (Intern)

Peuker, Dr.-Ing. Urs (Ekstern)

Project Manager, organisational:

Mørup, Steen (Intern)

Financing sources

Source: Private funding (private)
Name of research programme: Uddannelse. Private. Fonde  
Amount: 50,000.00 Danish Kroner

Project

Towards self-organized magnetic materials

Department of Physics

Center for Nanoteknologi

Period: 01/09/2005 → 31/03/2009

Number of participants: 1

Project ID: 20215

Project Manager, organisational:  
Frandsen, Cathrine (Intern)

Financing sources

Source: Forskningsrådene - Andre

Name of research programme: Forskningsrådene - Andre  
Amount: 2,000,000.00 Danish Kroner

Project

Center for Individual Nanoparticle Functionality

The main objective of the center is to explore and understand the fundamental relations between surface morphology and reactivity on the nanometer scale. A combination of new experimental initiatives supported by theoretical approaches will be employed. The primary objectives of the center are: * To establish a close and unambiguous correlation between the morphology and the reactivity, ultimately of experimental approaches and methods. * To challenge the widely held belief that there are chemical reactions catalyzed by metal surfaces, which are structure insensitive, i.e., without a strong dependence on the detailed atomic structure of the surface. * To develop a new concept where nanodstructures can catalyze chemical reactions under non-thermal conditions, operating on entirely different physical principles than current technology.

Experimental Surface and Nanomaterials Physics

Department of Physics

Department of Micro- and Nanotechnology

Department of Chemical and Biochemical Engineering

Center for Individual Nanoparticle Functionality

Haldor Topsoe AS

Technical University of Munich

Eindhoven University of Technology

Chalmers University of Technology

Period: 01/08/2005 → 31/07/2010

Number of participants: 5

Acronym: CINF

Project ID: 20211

Project participant:  
Nielsen, Jane Hvolbæk (Intern)

Quaade, Ulrich (Intern)

Schiøtz, Jakob (Intern)

Hansen, Ole (Intern)

Project Manager, organisational:  
Chorkendorff, Ib (Intern)

Financing sources

Source: Forsk. Andre statslige danske - Grundforskn.fonden

Name of research programme: Forsk. Andre statslige danske - Grundforskn.fonden  
Amount: 36,000,000.00 Danish Kroner

Project
CH4 Oxidation on Supported Gold Catalysts

Department of Physics
Period: 01/08/2005 → 05/11/2008
Number of participants: 5
Phd Student:
Walther, Guido (Intern)
Supervisor:
Quaade, Ulrich (Intern)
Main Supervisor:
Horch, Sebastian (Intern)
Examiner:
Hansen, Ole (Intern)
Rupprechter, Günther (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Programbevilling
Project: PhD

Design of Novel Materials for Energy Storage

Department of Physics
Period: 01/08/2005 → 02/02/2009
Number of participants: 6
Phd Student:
Voss, Johannes (Intern)
Supervisor:
Vegge, Tejs (Intern)
Main Supervisor:
Nørskov, Jens Kehlet (Intern)
Examiner:
Jacobsen, Karsten Wedel (Intern)
Jónsson, Hannes (Ekstern)
Manninen, Matti Jussi (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Risø (Løn)
Project: PhD

Direkte syntese af metanol fra metan

Department of Physics
Haldor Topsoe AS
Period: 01/08/2005 → 31/07/2006
Number of participants: 2
Project ID: 20230
Project Participant:
Abild-Pedersen, Frank (Intern)
Project Manager, organisational:
Nørskov, Jens Kehlet (Intern)

Financing sources
Source: Samarb.aftaler, Private danske - Andre virksomheder
Name of research programme: Samarb.aftaler, Private danske - Andre virksomheder
Amount: 539,000.00 Danish Kroner
Project

Fremstilling og test af tunnel-elektroner til forøgelse af overfladereaktivitet
Department of Physics
Period: 01/08/2005 → 10/02/2010
Number of participants: 6
Phd Student:

Nielsen, Gunver (Intern)
Supervisor:
Hansen, Ole (Intern)
Main Supervisor:
Chorkendorff, Ib (Intern)
Examiner:
Nielsen, Jane Hvolbæk (Intern)
Hornekær, Liv (Ekstern)
McFarland, Eric W. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-lønnet stipendie
Project: PhD

Johannes Voss
Department of Physics
Center for Nanoteknologi
Period: 01/08/2005 → 31/07/2008
Number of participants: 1
Project ID: 20221
Project Manager, organisational:
Nørskov, Jens Kehlet (Intern)

Financing sources
Source: Sektorforskningen - RISØ
Name of research programme: Sektorforskningen - RISØ
Amount: 288,000.00 Danish Kroner
Project

Modellering af biologiske processer i forbindelse med Parkinsons syge
Department of Physics
Period: 01/08/2005 → 28/11/2008
Number of participants: 5
Phd Student:

Mazin, Viktor (Intern)
Main Supervisor:
Mosekilde, Erik (Intern)
Examiner:
Berg-Sørensen, Kirstine (Intern)
Arvastson, Lars Johan (Intern)
Braun, Hans Albert (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU, Samfinansiering
Project: PhD

MD-Computer Simulations and Vibrational Spectroscopic Studies of Lipid-Protein Interactions: The Role of Interfacial Aromatic Residues
Department of Physics
Period: 01/07/2005 → 10/02/2010
Number of participants: 6
Phd Student:
Petersen, Frederic Nicolas Rønne (Intern)
Supervisor:
Hélix-Nielsen, Claus (Intern)
Main Supervisor:
Bohr, Tomas (Intern)
Examiner:
Berg-Sørensen, Kirstine (Intern)
Kleinschmidt, Jörg Helmut (Ekstern)
Westh, Peter (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-lønnet stipendie
Project: PhD

Nye funktionelle nanorør

Department of Physics
Period: 15/06/2005 → 03/09/2008
Number of participants: 6
Phd Student:
Strange, Mikkel (Intern)
Supervisor:
Thygesen, Kristian Sommer (Intern)
Main Supervisor:
Jacobsen, Karsten Wedel (Intern)
Examiner:
Schiøtz, Jakob (Intern)
Puska, Martti Juhani (Ekstern)
Stokbro, Kurt (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Programbevilling
Project: PhD

Towards 25% Efficiency Solar Cells: Modelling and Controlling Defects in Float Zone Silicon

Department of Physics
Period: 01/06/2005 → 30/04/2007
Number of participants: 2
Phd Student:
Kaat, Gregers Alexander (Intern)
Main Supervisor:
Schiøtz, Jakob (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Programbevilling
Project: PhD

Molekylære kontakters struktur, dynamik og transport

Department of Physics
Period: 01/03/2005 → 16/12/2009
Number of participants: 6
Phd Student:
Bækgaard, Iben Sig Buur (Intern)
Supervisor:
Thygesen, Kristian Sommer (Intern)
Nanopartikler af antiferromagnetiske materialer

Department of Physics
Period: 01/03/2005 → 29/09/2008
Number of participants: 6
Phd Student:
Madsen, Daniel Esmarch (Intern)
Supervisor:
Hansen, Mikkel Fougt (Intern)
Main Supervisor:
Mørup, Steen (Intern)
Examiner:
Jacobsen, Claus Schelde (Intern)
Pierre, Tim St. (Ekstern)
Wäppling, Roger (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-lønnet stipendie
Project: PhD

Towards 25% efficiency solar cells: modelling and controlling defects in zone silicon
The main objectives of the projects: 1. To develop a software for computer simulation of grown-in vacancy defects and impurities formed in monocrystalline silicon grown by float zone technique. 2. To establish a correlation between impurities and vacancy type defects and carrier lifetime which is the key material parameter for solar cell silicon. 3. To provide input for control of the distribution of impurities and grown-in vacancy defects in monocrystalline float zone silicon in order to optimise carrier lifetime and solar cell efficiency.

Department of Physics
Center for Individual Nanoparticle Functionality
Topsil Semiconductor Materials A/S
Period: 01/03/2005 → 31/03/2008
Number of participants: 1
Project ID: 20198
Project Manager, organisational:
Schiøtz, Jakob (Intern)

Financing sources
Source: Forskningsrådsfinansiering
Name of research programme: Forskningsrådsfinansiering
Amount: 2,427,000.00 Danish Kroner
Project

Anca Paduraru C:O:N:T samarbejde
Collaboration with Nano Science Center at the University of Copenhagen.

Department of Physics
Center for Nanoteknologi
Plastic Deformation of Metallic Glasses

Department of Physics
Period: 01/02/2005 → 31/03/2008
Number of participants: 6
PhD Student:
Paduraru, Anca (Intern)
Supervisor:
Schiøtz, Jakob (Intern)
Main Supervisor:
Jacobsen, Karsten Wedel (Intern)
Examiner:
Nørskov, Jens Kehlet (Intern)
Evangelakis, Giorgos (Ekstern)
Wahnström, Göran (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 DTU-stip, 2/3 FUR/andet
Project: PhD

Nye elektrode materialer til hydrogen produktion

Department of Physics
Period: 15/01/2005 → 02/07/2008
Number of participants: 5
PhD Student:
Bonde, Jacob Lindner (Intern)
Main Supervisor:
Chorkendorff, I (Intern)
Supervisor:
Schiøtz, Jakob (Intern)
Alonso-Vante, Nicolás (Ekstern)
Stimming, Ulrich (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Programbevilling
Project: PhD

Fluid Dynamics of Living Systems

Department of Physics
Period: 07/01/2005 → 31/12/2007
Number of participants: 1
Project ID: 20199
Project Manager, organisational:
Bohr, Tomas (Intern)

Financing sources
Danish Center for Scientific Computing (DCSC) - 3

Department of Physics
Period: 01/01/2005 → 01/06/2006
Number of participants: 1
Project ID: 20203
Project Manager, organisational:
Jacobsen, Karsten Wedel (Ekstern)

Financing sources
Source: Forskningsprojekter - Andre ministerier og styrelser
Name of research programme: Forskningsprojekter - Andre ministerier og styrelser
Amount: 600,000.00 Danish Kroner

Design of functional nanomaterials
To establish a research collaboration encompassing all steps in the development of new functional nanomaterials: design, synthesis, characterization, and testing. The common aim of the proposal is the development of rational design strategies for nano-structured materials.

Department of Physics
Department of Chemistry
Administration
Department of Chemical and Biochemical Engineering
Department of Micro- and Nanotechnology
Risø National Laboratory for Sustainable Energy
Center for Individual Nanoparticle Functionality
Center for Nanoteknologi
Period: 01/01/2005 → 31/12/2008
Number of participants: 19
Project ID: 20195
Project participant:
Jacobsen, Karsten Wedel (Intern)
Chorkendorff, Ib (Intern)
Nielsen, Jane Hvolbæk (Intern)
Horch, Sebastian (Intern)
Schiøtz, Jakob (Intern)
Hansen, Jørn Bindslev (Ekstern)
Quaade, Ulrich (Intern)
Christensen, Claus H. (Intern)
Ulstrup, Jens (Intern)
Johannessen, Tue (Intern)
Bøggild, Peter (Intern)
Pedersen, Allan Schröder (Intern)
Mogensen, Mogens (Intern)
Vegge, Tejs (Intern)
Pryds, Nini (Intern)
Henriksen, Peter Vang (Ekstern)
Kuhn, Luise Theil (Intern)
**Heterogeneous catalysis for chemical production**

Catalysis is one of the technological pillars of modern chemical industry. Catalysis also holds the key to the solution of many environmental and energy problems. The challenge in the field is to devise new methods that can accelerate the development of new catalysts and processes beyond the intuitive trial-and-error approach. It is suggested to form a collaborative program encompassing the whole range from computational design and experimental analysis of model systems to synthesis and testing of new catalysts. The aim of the program is to develop new tools allowing for the rational design of catalysts and catalytic processes for chemical industry and for environmental protection.

Department of Physics

Department of Chemistry

Department of Chemical and Biochemical Engineering

Center for Nanoteknologi

Haldor Topsoe AS

University of Iceland

Period: 01/01/2005 → 31/12/2009

Number of participants: 5

Project ID: 20194

**Investigation of Non-Classical Light and its Application in Ultra-Sensitive Measurements**

Department of Physics

Period: 01/01/2005 → 30/04/2008

Number of participants: 5

Phd Student:

Janousek, Jirí (Intern)

Main Supervisor:

Buchhave, Preben (Intern)

Examiner:

Hald, Jan (Ekstern)

Filip, Radim (Ekstern)

Schnabel, Roman (Ekstern)

**Financing sources**

Source: Internal funding (public)

Name of research programme: 1/3 DTU-stip, 2/3 FUR/andet

Project: PhD
New electrode materials for hydrogen production

It is proposed to explore the potential of a recent invention where a new class of materials has been identified as electrodes for hydrogen evolution. Presently platinum and other extremely expensive noble metals are the best electrode materials, and it is essential for a possible future hydrogen economy to find cheaper and equally efficient replacements. Our approach involves a search for new and more efficient variations of a new class of materials based on transition metal sulfides. We will be exploiting the synergy between designs on the basis of electronic structure calculations and the synthesis and testing of new materials.

Department of Physics

Department of Chemical and Biochemical Engineering

Center for Individual Nanoparticle Functionality

IRD Fuel Cells A/S

Financing sources

Source: Forskningsrådene - Andre
Name of research programme: Forskningsrådene - Andre
Amount: 3,600,000.00 Danish Kroner
Using DFT to screen for new catalysts for Fischer Tropsch synthesis: EU Fellowship

(a) Gain improved insight into the detailed mechanisms of Fischer-Tropsch catalysts: It is now well known that high pressures of CO and H2 induces large structural changes to the catalytic surface and that these self-organized surface structures are in fact responsible for the catalytic activity. Despite all experimental work on the subject, no entirely satisfactory reaction mechanism has been proposed, and in particular the parameters determining the selectivity of the catalyst are unknown. It is our belief that by detailed investigation of these systems using density functional calculations, we are going to be able to deduce details of the actual reaction mechanism and pinpoint the most important parameters determining the activity and more importantly the selectivity of the currently used catalysts. (b) Screening for new possible Fischer-Tropsch catalysts using DFT: With detailed knowledge on parameters determining the selectivity we will use density functional theory for a very wide range of materials in a search for catalyst candidates that exhibit the desired properties, i.e. are highly selective towards desired reaction products. For catalyst materials exhibiting similar selectivity we expect to find materials capable of working at lower temperatures and/or that are less prone to poisoning effects and/or that have better stability in time. Finding materials with properties indicating a very high selectivity is very important as controlling the selectivity will allow for much greater reaction yield for the desired final products. (c) Synthesis and characterization of new materials: Through collaboration with Prof. Christensen at the Department of Chemistry at the Technical University of Denmark we will try to synthesise the proposed catalyst materials and investigate their catalytic activity, both by kinetic evaluation and by in-situ techniques. By combining their experimental data with further computer simulations we hope to refine our search and further improve the properties of the proposed catalytic materials. It is important to point out that this part of the project involves close collaboration between theory and experiment, since a combined search more often than not is more successful than an isolated theoretical or experimental study.
Christensen, Claus H. (Ekstern)
Main Supervisor:
Nørskov, Jens Kehlet (Intern)
Examiner:
Jacobsen, Karsten Wedel (Intern)
Hu, Peijun (Ekstern)
Maier, Wilhelm F. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 DTU-stip, 2/3 FUR/andet
Project: PhD

Ture Rønved Munter ph.d.-projekt
Department of Physics
Period: 01/10/2004 → 31/12/2007
Number of participants: 1
Project ID: 20184
Project Manager, organisational:
Nørskov, Jens Kehlet (Ekstern)

Financing sources
Source: Ph.d. Institut finansieret
Name of research programme: Ph.d. Institut finansieret
Amount: 1,500,000.00 Danish Kroner
Project

Modifikation af kobber på nano-skala-nievau til udvikling af nye metanol- og WGS-katalysatører
Department of Physics
Period: 01/08/2004 → 31/01/2008
Number of participants: 6
Phd Student:
Schumacher, Nana Maria Pii (Intern)
Supervisor:
Nerlov, Jesper (Intern)
Main Supervisor:
Chorkendorff, Ib (Intern)
Examiner:
Horch, Sebastian (Intern)
Hinrichsen, Kai-Olaf (Ekstern)
Nakamura, Junji (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 DTU-stip, 2/3 FUR/andet
Project: PhD

Nana Schumacher ph.d.-projekt
Department of Physics
Period: 01/08/2004 → 31/10/2007
Number of participants: 1
Project Manager, organisational:
Chorkendorff, Ib (Ekstern)

Financing sources
Source: Ph.d. Institut finansieret
Name of research programme: Ph.d. Institut finansieret
Amount: 1,500,000.00 Danish Kroner
Project
Peter B. Mozhaev

Department of Physics
Period: 25/06/2004 → 31/08/2005
Number of participants: 3
Project ID: 20185
Project participant:
Mozhaev, Peter (Intern)
Mozhaeva, Julia (Intern)

Project Manager, organisational:
Jacobsen, Claus Schelde (Intern)

Financing sources
Source: Uddannelse. Private. Andre virksomheder
Name of research programme: Uddannelse. Private. Andre virksomheder
Amount: 50,000.00 Danish Kroner

Yuri Gaidideis gasteprofessorat

Department of Physics
Period: 25/06/2004 → 31/03/2005
Number of participants: 1
Project ID: 20186
Project Manager, organisational:
Mosekilde, Erik (Intern)

Financing sources
Source: Gaver, Private danske Fonde
Name of research programme: Gaver, Private danske Fonde
Amount: 100,000.00 Danish Kroner

Synchronization of Nephrons in the Kidneys of Normotensive and Hypertensive Rats

Department of Physics
Period: 30/04/2004 → 31/05/2005
Number of participants: 2
Project participant:
Sosnovtseva, Olga (Intern)
Project Manager, organisational:
Mosekilde, Erik (Intern)

Financing sources
Source: Gaver, Private danske Fonde
Name of research programme: Gaver, Private danske Fonde
Amount: 870,000.00 Danish Kroner

Investigation of Non-classical Light

Department of Physics
Period: 01/04/2004 → 31/03/2007
Number of participants: 1
Project ID: 20171
Project Manager, organisational:
Buchhave, Preben (Intern)

Financing sources
Source: Forskningsrådene - STVF
Name of research programme: Forskningsrådene - STVF
Amount: 1,700,000.00 Danish Kroner
Investigation of Non-Classical Light and its Applications in Biomedical Measurements and Imaging

Department of Physics
Period: 01/04/2004 → 01/08/2007
Number of participants: 4
Phd Student:
Lassen, Mikael Østergaard (Intern)
Main Supervisor:
Buchhave, Preben (Intern)
Examiner:
Schnabel, Roman (Ekstern)
Thomsen, Jan Westenkaer (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Studie af bevidsthed og intelligens

Department of Physics
Period: 25/03/2004 → 31/12/2004
Number of participants: 1
Project ID: 20179
Project Manager, organisational:
Cotterill, Rodney M J (Intern)

Financing sources
Source: Gaver, Private danske Fonde
Name of research programme: Gaver, Private danske Fonde
Amount: 30,000.00 Danish Kroner

Semiconductor Components for Quantum Informatics

Department of Physics
Period: 17/03/2004 → 31/03/2007
Number of participants: 1
Project ID: 20178
Project Manager, organisational:
Hansen, Jørn Bindslev (Ekstern)

Financing sources
Source: Forskningsrådene - SNF
Name of research programme: Forskningsrådene - STVF
Amount: 100,000.00 Danish Kroner

Undersøgelse af nanopartiklers morfologi med skanning tunnel mikroskopi

Department of Physics
Period: 01/03/2004 → 01/08/2007
Number of participants: 5
Phd Student:
Jørgensen, Kristina Pilt (Intern)
Main Supervisor:
Nielsen, Jane Hvolbæk (Intern)
Examiner:
Hansen, Ole (Intern)
Diekhöner, Lars (Ekstern)
Spectroscopic Studies of Cytochrome P450 Enzymes by Application of Optical Spectroscopic Techniques Combined with QM/MM Calculations

Department of Physics
Period: 01/02/2004 → 01/08/2007
Number of participants: 6
Phd Student:
Johannessen, Christian (Intern)
Supervisor:
Abdali, Salim (Intern)
Main Supervisor:
Bohr, Henrik (Intern)
Examiner:
Rottwitt, Karsten (Intern)
Blanch, Ewan William (Ekstern)
Ramanujam, P.S. (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-lønnet stipendie
Project: PhD

Danish Center for Scientific Computing (DCSC) - 2
Installation and operation of a Linux cluster. The machine is dedicated to ambitious research projects within material physics, heterogeneous catalysis and electrochemistry.

Department of Physics
Period: 01/01/2004 → 31/12/2007
Number of participants: 1
Project ID: 20172
Project Manager, organisational:
Jacobsen, Karsten Wedel (Intern)

Financing sources
Source: Forsk. Private danske - Andre
Name of research programme: Forsk. Private danske - Andre
Amount: 4,000,000.00 Danish Kroner
Project
**Ductile BMG Composites**

Bulk metallic glasses are an exciting new class of materials with high yield stress and low elastic moduli, making them interesting in situations where mechanical energy is stored (springs etc). Unfortunately, they are quite brittle, and fail through the formation of shear bands. We use molecular dynamics simulations to study the deformation mechanisms and shear band formation with the goal of designing less brittle metallic glasses.

Department of Physics

Center for Nanoteknologi

Centre National de la Recherche Scientifique

University of Cambridge

Leibniz Institute for Solid State and Materials Research Dresden

Universität Ulm

European Synchrotron Radiation Facility

Universidad Autonoma de Barcelona

Polskiej Akademii Nauk

University of Turin

Waterford Institute of Technology

University of Ioannina

Period: 01/01/2004 → 31/12/2008

Number of participants: 3

Project ID: 20177

Contact person:

Yavari, Reza (Ekstern)

Project participant:

Schiøtz, Jakob (Intern)

Project Manager, organisational:

Jacobsen, Karsten Wedel (Intern)

**Financing sources**

Source: Forsk. EU - Rammeprogram

Name of research programme: Forsk. EU - Rammeprogram

Amount: 1,529,600.00 Danish Kroner

**Postdoc employment, Stadler**

Department of Physics

Period: 01/01/2004 → 31/12/2006

Number of participants: 1

Project ID: 20165

Project Manager, organisational:

Jacobsen, Karsten Wedel (Ekstern)

**Financing sources**

Source: Forskningsprojekter - Andre ministerier og styrelser

Name of research programme: Forskningsprojekter - Andre ministerier og styrelser

Amount: 1,000,000.00 Danish Kroner

**Improved THz-Band SIR**

Department of Physics

Period: 10/10/2003 → 30/06/2004

Number of participants: 1

Project Manager, organisational:

Mygind, Jesper (Intern)
Financing sources
Source: Sam.arb.aftaler - Udenlandske offentlige og private
Name of research programme: Sam.arb.aftaler - Udenlandske offentlige og private
Amount: 99,950.00 Danish Kroner

Dmitry Postnov
Department of Physics
Period: 09/10/2003 → 31/12/2004
Number of participants: 2
Project participant:
Postnov, Dmitry (Ekstern)
Project Manager, organisational:
Mosekilde, Erik (Intern)

Financing sources
Source: Gaver, Private danske Fonde
Name of research programme: Gaver, Private danske Fonde
Amount: 216,000.00 Danish Kroner

Højtemperatureslektrolyse
Department of Physics
Period: 01/10/2003 → 08/02/2007
Number of participants: 7
Phd Student:
Jensen, Søren Højgaard (Intern)
Supervisor:
Hendriksen, Peter Vang (Intern)
Mogensen, Mogens Bjerg (Intern)
Main Supervisor:
Chorkendorff, Ib (Intern)
Examiner:
Skaarup, Steen (Intern)
Ivers-Tiffée, Ellen (Ekstern)
Skou, Eivind Morten (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Risø (Løn)
Project: PhD

Søren Højgaard Jensen
Department of Physics
Period: 01/10/2003 → 30/09/2006
Number of participants: 1
Project ID: 20163
Project Manager, organisational:
Chorkendorff, Ib (Ekstern)

Financing sources
Source: Sektorforskningen - RISØ
Name of research programme: Sektorforskningen - RISØ
Amount: 270,180.00 Danish Kroner

Biosimulation - A New Tool in Drug Development
Department of Physics
Period: 16/09/2003 → 30/06/2004  
Number of participants: 2  
Project participant:  
Sosnovtseva, Olga (Intern)  
Project Manager, organisational:  
Moskilde, Erik (Intern)  

**Financing sources**  
Source: Forskningsrådene - Andre  
Name of research programme: Forskningsrådene - Andre  
Amount: 117,000.00 Danish Kroner  
Project

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**Måling af hurtige ioners dynamik i fusions plasmaer ved hjælp af kollektiv Thomson spredning (CTS)**  
Department of Physics  
Period: 01/09/2003 → 13/12/2007  
Number of participants: 6  
Phd Student:  
Nielsen, Stefan Kragh (Intern)  
Supervisor:  
Bindslev, Henrik (Intern)  
Main Supervisor:  
Bohr, Tomas (Intern)  
Examiner:  
Hansen, Jørn Otto Bindslev (Ekstern)  
Hartfus, Hans-Jürgen (Ekstern)  
Kasperek, Walter (Ekstern)  

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Risø (Len)  
Project: PhD

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**Udvikling af algoritmer til direkte-rum elektronstrukturberegninger på massivt parallele computere**  
Department of Physics  
Period: 01/09/2003 → 31/08/2005  
Number of participants: 1  
Project ID: 20140  
Project Manager, organisational:  
Mortensen, Jens Jørgen (Ekstern)  

**Financing sources**  
Source: Gaver, Private danske Fonde  
Name of research programme: Gaver, Private danske Fonde  
Amount: 862,500.00 Danish Kroner  
Project

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**Størrelsesseffekter ved anvendelse af nanopartikler til brintlagering**  
Department of Physics  
Number of participants: 6  
Phd Student:  
Engbæk, Jakob (Intern)  
Supervisor:  
Nielsen, Jane Hvolbæk (Intern)  
Main Supervisor:  
Chorkendorff, Ib (Intern)  
Examiner:  
Quaade, Ulrich (Intern)
Niemantsverdriet, J. W. Hans (Ekstern)
Sehested, Jens (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: DTU-lønnet stipendie
Project: PhD

**Bestemmelse af absolut konfiguration af chirale molekyler ved anvendelse af vibrationel cirkulær dichroisme (VCD) spektroskopi**

Department of Physics
Number of participants: 7
Phd Student:
Lassen, Peter Rygaard (Intern)
Supervisor:
Hemmingsen, Lars Bo Stegeager (Intern)
Norrby, Per-Ola (Intern)
Main Supervisor:
Bohr, Henrik (Intern)
Examiner:
Henriksen, Niels Engholm (Intern)
Bour, Petr (Ekstern)
Larsen, Leif Erik (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: DTU-lønnet stipendie
Project: PhD

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**Christian Bahl**

Department of Physics
Period: 01/07/2003 → 30/06/2006
Number of participants: 1
Project ID: 20159
Project Manager, organisational:
Mørup, Steen (Ekstern)

**Financing sources**
Source: Sektorforskningen - RISØ
Name of research programme: Sektorforskningen - RISØ
Amount: 270,180.00 Danish Kroner
Project

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**Magnetiske Nanopartikler og Nanokompositmaterialer**

Department of Physics
Number of participants: 7
Phd Student:
Bahl, Christian (Intern)
Supervisor:
Kuhn, Luise Theil (Intern)
Lefmann, Kim (Intern)
Main Supervisor:
Mørup, Steen (Intern)
Examiner:
Jacobsen, Claus Schelde (Intern)
Pankhurst, Quentin Andrew (Ekstern)
Zabel, Hartmut (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Risø (Løn)
Project: PhD

**Tunbare lasere i det synlige og ultraviolette område**
Department of Physics
Period: 01/06/2003 → 20/11/2006
Number of participants: 6
Phd Student: Mortensen, Jesper Liltorp (Intern)
Supervisor: Buchhave, Preben (Intern)
Main Supervisor: Tidemand-Lichtenberg, Peter (Intern)
Examiner: Lodahl, Peter (Intern)
Arie, Ady (Ekstern)
Petersen, Paul Michael (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

**Functional Dynamics in Complex Biosystems**
Department of Physics
Period: 30/05/2003 → 31/12/2004
Number of participants: 1
Project Manager, organisational: Mosekilde, Erik (Intern)

**Financing sources**
Source: Forskningsrådene - SNF
Name of research programme: Forskningsrådene - STVF
Amount: 200,000.00 Danish Kroner
Project

**Bulk Metallic Glass II**
Department of Physics
Period: 06/05/2003 → 30/06/2004
Number of participants: 1
Project Manager, organisational: Jiang, Jianzhong (Intern)

**Financing sources**
Source: Uddannelse. Statslige. Andre statslige
Name of research programme: Uddannelse. Statslige. Andre statslige
Amount: 75,000.00 Danish Kroner
Project

**Konstruktion og anvendelse af kryogen nanomotor med atomar positionering**
Department of Physics
Period: 01/05/2003 → 01/12/2005
Number of participants: 2
Phd Student:
Thomsen, Benjamin (Intern)
Main Supervisor:
Mygind, Jesper (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-lønnet stipendie
Project: PhD

Peter B. Mozhaev
Department of Physics
Period: 07/04/2003 → 31/05/2004
Number of participants: 2
Project participant:
Mozhaev, Peter (Intern)
Project Manager, organisational:
Jacobsen, Claus Schelde (Intern)

Financing sources
Source: Uddannelse. EU. Andre EU-midler
Name of research programme: Uddannelse. EU. Andre EU-midler
Amount: 15,000.00 Danish Kroner
Project

Forskerudveksling fra Japan
Department of Physics
Osaka University
Period: 01/04/2003 → 31/03/2004
Number of participants: 2
Project ID: 20149
Project participant:
Morikawa, Yoshitada (Intern)
Project Manager, organisational:
Nørskov, Jens Kehlet (Intern)

Financing sources
Source: Uddannelse. Statslige. Andre statslige
Name of research programme: Uddannelse. Statslige. Andre statslige
Amount: 591,332.00 Danish Kroner
Project

Ultra-Low-Noise
Department of Physics
Period: 11/02/2003 → 31/03/2005
Number of participants: 1
Project Manager, organisational:
Mygind, Jesper (Intern)

Financing sources
Source: Forsk. EU - Rammeprogram
Name of research programme: Forsk. EU - Rammeprogram
Amount: 44,580.00 Danish Kroner
Project

Crystallisation kinetics
Department of Physics
Period: 04/02/2003 → 30/04/2004
Number of participants: 1
Project Manager, organisational:
Jiang, Jianzhong (Intern)

**Financing sources**
Source: Uddannelse. Private. Andre virksomheder
Name of research programme: Uddannelse. Private. Andre virksomheder
Amount: 75,000.00 Danish Kroner

**Room Temperature Magnetic Semiconductors for Spintronic Field Effect Transistors**

Department of Physics
Period: 01/02/2003 → 07/09/2006
Number of participants: 7
Phd Student:
Damsgaard, Christian Danvad (Intern)
Supervisor:
Jacobsen, Claus Schelde (Intern)
Lindelof, Poul Erik (Intern)
Main Supervisor:
Hansen, Jørn Otto Bindslev (Ekstern)
Examiner:
Hvam, Jørn Marcher (Intern)
Foxon, Charles Thomas Bayley (Ekstern)
Ploog, Klaus H. (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Karen Y. Constantinian

Department of Physics
Period: 31/01/2003 → 29/12/2003
Number of participants: 2
Project participant:
Constantinian, Karen (Ekstern)
Project Manager, organisational:
Mygind, Jesper (Intern)

**Financing sources**
Source: Uddannelse. EU. Andre EU-midler
Name of research programme: Uddannelse. EU. Andre EU-midler
Amount: 15,000.00 Danish Kroner

**Flammesyntetiserede katalysatorer i mikroreaktorer**

Department of Physics
Period: 01/01/2003 → 31/12/2004
Number of participants: 1
Project ID: 20142
Project Manager, organisational:
Quaade, Ulrich (Ekstern)

**Financing sources**
Source: Forskningsrådene - STVF
Name of research programme: Forskningsrådene - STVF
Amount: 1,130,000.00 Danish Kroner
Lyskilder til ikke-invasive to-foton processer i øjet

Department of Physics
Period: 01/01/2003 → 31/05/2007
Number of participants: 7
Phd Student:
Thorhauge, Morten (Intern)
Supervisor:
Buchhave, Preben (Intern)
Larsen, Michael (Ekstern)
Main Supervisor:
Tidemand-Lichtenberg, Peter (Intern)
Examiner:
Rottwitt, Karsten (Intern)
Laurell, Fredrik (Ekstern)
Sander, Birgit Agnes (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-lønned stipendie
Project: PhD

New Metal Hydrides for Energy Storage

Department of Chemistry
Department of Physics
Institute for Energy Technology
Stockholm University
University of Oslo
Lithuanian Energy Institute
Helsinki University of Technology
Period: 01/01/2003 → 31/12/2006
Number of participants: 8
Project ID: 62-02
Project participant:
Jensen, Jens Oluf (Intern)
Noréus, Dag (Ekstern)
Fjellvåg, Helmer (Ekstern)
Noréus, Dag (Ekstern)
Milcic, Darius (Ekstern)
Lampinen, Markku J. (Ekstern)
Project Manager, organisational:
Bjerrum, Niels J. (Intern)
Hauback, Bjørn C. (Ekstern)

Financing sources
Source: Forsk. Andre offentlige og private - Nordiske
Name of research programme: Forsk. Andre offentlige og private - Nordiske
Amount: 500,000.00 Danish Kroner
Project

Integrated Superconducting Spectrometer

Department of Physics
Period: 17/12/2002 → 31/12/2006
Number of participants: 1
**Financing sources**

Source: Forsk. EU - Rammeprogram  
Name of research programme: Forsk. EU - Rammeprogram  
Amount: 59,440.00 Danish Kroner  

**Øresundsbevilling**

Department of Physics  
Number of participants: 1  
Project ID: 20137  
Project Manager, organisational:  
Mørup, Steen (Ekstern)  

**Financing sources**

Source: Uddannelse, udenlandske offentlige og private  
Name of research programme: Uddannelse, udenlandske offentlige og private  
Amount: 25,000.00 Danish Kroner  

**Øresundsuniversitetet**

Department of Physics  
Number of participants: 1  
Project Manager, organisational:  
Mørup, Steen (Intern)  

**Financing sources**

Source: Uddannelse, udenlandske offentlige og private  
Name of research programme: Uddannelse, udenlandske offentlige og private  
Amount: 24,970.00 Danish Kroner  

**THz-Band Superconducting**

Department of Physics  
Period: 24/10/2002 → 29/12/2003  
Number of participants: 2  
Project participant:  
Prokopenko, Georgy (Ekstern)  
Project Manager, organisational:  
Mygind, Jesper (Intern)  

**Financing sources**

Source: Forsk. Andre offentlige og private - Udenlandske  
Name of research programme: Forsk. Andre offentlige og private - Udenlandske  
Amount: 99,486.00 Danish Kroner  

**Parallel screening af potentielle legerings katalysatorer til dissociation af brint og reforming af methanol**

Department of Physics  
Period: 01/09/2002 → 02/01/2006  
Number of participants: 6  
Phd Student:  
Lytken, Ole (Intern)  
Supervisor:  
Dahl, Søren (Intern)
Main Supervisor:
Chorkendorff, Ib (Intern)
Examiner:
Nielsen, Jane Hvolbæk (Intern)
Sehested, Jens (Intern)
Valden, Mika O. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Synchronization of Biological Oscillators
Department of Physics
Period: 28/08/2002 → 31/08/2005
Number of participants: 1
Project Manager, organisational:
Mosekilde, Erik (Intern)

Financing sources
Source: Forsk. EU - Rammeprogram
Name of research programme: Forsk. EU - Rammeprogram
Amount: 26,640.00 Danish Kroner
Project

Superconducting structures
Department of Physics
Period: 10/07/2002 → 31/07/2006
Number of participants: 1
Project Manager, organisational:
Mygind, Jesper (Intern)

Financing sources
Source: Forsk. EU - Rammeprogram
Name of research programme: Forsk. EU - Rammeprogram
Amount: 52,000.00 Danish Kroner
Project

Microwave Oscillators with Low Phase Noise and Ultra-High Stability
Department of Physics
Period: 01/07/2002 → 07/09/2006
Number of participants: 7
Phd Student:
Basu, Ronni (Intern)
Supervisor:
Krozer, Viktor (Intern)
Pedersen, Peder (Ekstern)
Main Supervisor:
Mygind, Jesper (Intern)
Examiner:
Jacobsen, Claus Schelde (Intern)
Levinsen, Mogens Tveddell (Ekstern)
Liopis, Olivier (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU, Samfinansiering
Project: PhD
Predicting Catalysis: Understanding ammonia production from first principles

Department of Physics
Period: 01/07/2002 → 30/06/2006
Number of participants: 1
Project ID: 20134
Project Manager, organisational:
Nørskov, Jens Kehlet (Ekstern)

Financing sources
Source: Forsk. EU - Rammeprogram
Name of research programme: Forsk. EU - Rammeprogram
Amount: 1,499,800.00 Danish Kroner

Biomedicinsk optik og nye lasersystemer

Department of Physics
Period: 21/06/2002 → 31/12/2005
Number of participants: 1
Project Manager, organisational:
Buchhave, Preben (Intern)

Financing sources
Source: [Ordinær drift UK 10]
Name of research programme: [Ordinær drift UK 10]
Amount: 5,000,000.00 Danish Kroner

Metal-oxide thin film heterostructures

Department of Physics
Period: 21/06/2002 → 31/12/2005
Number of participants: 1
Project Manager, organisational:
Jacobsen, Claus Schelde (Intern)

Financing sources
Source: Forsk. EU - Rammeprogram
Name of research programme: Forsk. EU - Rammeprogram
Amount: 52,000.00 Danish Kroner

Fundamentale undersøgelser af dannelseskinetik og stabilitet af lette metalhydride

Department of Physics
Period: 01/06/2002 → 02/01/2006
Number of participants: 7
Phd Student:
Ostenfeld, Christopher Worsøe (Intern)
Supervisor:
Dahl, Søren (Intern)
Pedersen, Allan Schröder (Intern)
Main Supervisor:
Chorkendorff, Ib (Intern)
Examiner:
Quaade, Ulrich (Intern)
Jensen, Torben René (Ekstern)
Jónsson, Hannes (Ekstern)

Financing sources
**Towards a Hydrogen-based Society**

Experts stipulate that the world’s oil and gas resources will be emptied in less than a hundred years. Although the coal resources are significantly larger than those of oil and gas, coal cannot substitute oil and gas without severe environmental consequences. All major industrialized countries thus carry out intensive research to find clean and sustainable energy alternatives. Hydrogen is generally accepted as a possible future replacement of fossil fuels and it will play a crucial role as a new clean energy carrier. The vision of the so-called hydrogen society is to use renewable energy sources to produce hydrogen by simply dissociating water molecules. When the energy stored in hydrogen is converted into, e.g., electricity and heat in a fuel cell, water is formed again as the only by-product in a pollution-free and sustainable process. However, the technologies needed to realize this vision still require development and significant improvement before hydrogen presents a realistic alternative to the fossil fuel based energy system. To develop new schemes and improve existing technologies to produce and store hydrogen and to convert the energy in hydrogen to electricity, fundamental as well as more applied research must be performed. We propose the establishment of a large, interdisciplinary, inter-institutional research center with the main objective of carrying out research within the technologies associated with the hydrogen society. The center will comprise some of the most competent and internationally well-recognized research groups in Denmark within the proposed subjects. The balanced mix of fundamental research, carried
out mainly by the university groups, and the more applied research, carried out by the industrial partners and groups at a national research center, ensures that all important aspects from basic science to commercialization of the hydrogen technologies are treated. The specific objectives of the proposed project are to - perform research and development on electrode catalysts for two different types of fuel cells - perform research and development on hydrogen storage materials such as metal hydrides - demonstrate small energy units based on the hydrogen technology - evaluate the implementation and implications of the hydrogen technology in the society

Department of Physics
Rise National Laboratory for Sustainable Energy
Department of Chemical and Biochemical Engineering
Center for Individual Nanoparticle Functionality
Center for Nanoteknologi
Aarhus University
IRD Fuel Cells A/S
Haldor Topsoe AS
Danfoss A/S
Period: 05/03/2002 → 31/12/2006
Number of participants: 6
Project ID: 20112
Project participant:
Besenbacher, Flemming (Ekstern)
Hammer, Bjørk (Ekstern)
Pedersen, Allan Scrøder (Ekstern)
Andersen, Steen Yde (Ekstern)
Clausen, Bjerne S. (Ekstern)
Project Manager, organisational:
Chorkendorff, Ib (Intern)

Financing sources
Source: Forskningsrådene - STVF
Name of research programme: Forskningsrådene - STVF
Amount: 3,736,300.00 Danish Kroner

Måleudstyr til kvantekomponenter
Department of Physics
Period: 25/02/2002 → 31/10/2010
Number of participants: 1
Project Manager, organisational:
Mygind, Jesper (Intern)

Financing sources
Source: Gaver, Private danske Fonde
Name of research programme: Gaver, Private danske Fonde
Amount: 923,398.00 Danish Kroner

Danish Center for Scientific Computing (DCSC) - 1
Department of Physics
Period: 18/02/2002 → 25/08/2003
Number of participants: 1
Project ID: 20110
Project Manager, organisational:
Jacobsen, Karsten Wedel (Ekstern)

Financing sources
Source: Forskningsprojekter - Andre ministerier og styrelser
Name of research programme: Forskningsprojekter - Andre ministerier og styrelser
Amount: 6,100,000.00 Danish Kroner
Project

**Metan aktivering**

Department of Physics  
Period: 01/02/2002 → 28/09/2005  
Number of participants: 4  
Phd Student: Abild-Pedersen, Frank (Intern)  
Main Supervisor: Nørskov, Jens Kehlet (Intern)  
Examiner: Jacobsen, Karsten Wedel (Intern)  
Lundqvist, Bengt I. (Ekstern)

**Financing sources**

Source: Internal funding (public)
Name of research programme: Grundforskningsfonden
Project: PhD

**Nanomag**

Department of Physics  
Period: 01/02/2002 → 31/07/2004  
Number of participants: 1  
Project Manager, organisational: Jiang, Jianzhong (Intern)

**Financing sources**

Source: Forsk. EU - Rammeprogram  
Name of research programme: Forsk. EU - Rammeprogram  
Amount: 300,000.00 Danish Kroner
Project

**Nanostrukturers opbygning, dynamik og transportegenskaber**

Department of Physics  
Period: 01/02/2002 → 06/06/2005  
Number of participants: 5  
Phd Student: Thygesen, Kristian Sommer (Intern)  
Main Supervisor: Jacobsen, Karsten Wedel (Intern)  
Examiner: Nørskov, Jens Kehlet (Intern)  
Gonze, Xavier (Ekstern)  
Stokbro, Kurt (Intern)

**Financing sources**

Source: Internal funding (public)  
Name of research programme: DTU-lønnet stipendie  
Project: PhD

**Artificial Consciousness and Intelligence**

Department of Physics  
Period: 16/01/2002 → 30/06/2004  
Number of participants: 1  
Project Manager, organisational: Cotterill, Rodney M J (Intern)
### Advanced PEM Fuel Cells (APOLLON)

**Department of Physics**

- **Period:** 01/12/2001 → 30/11/2004
- **Number of participants:** 1
- **Project ID:** 20107
- **Project Manager, organisational:** Nørskov, Jens Kehlet (Ekstern)

**Financing sources**

- **Source:** Forskningsrådene - SNF
- **Name of research programme:** Forskningsrådene - STVF
- **Amount:** 100,000.00 Danish Kroner

**Project**

### A protein-system investigated by NMR/ESR

**Department of Physics**

- **Period:** 01/12/2001 → 18/04/2006
- **Number of participants:** 6
- **PhD Student:** Jürgensen, Vibeke Würtz (Intern)
- **Supervisor:** Poulsen, Flemming (Ekstern)
- **Main Supervisor:** Bohr, Henrik (Intern)
- **Examiner:**
  - Christensen, Hans Erik Mølager (Intern)
  - Hemmingsen, Lars Bo Stegeager (Intern)
  - Redfield, Christina (Ekstern)

**Financing sources**

- **Source:** Forsk. EU - Rammeprogram
- **Name of research programme:** Forsk. EU - Rammeprogram
- **Amount:** 2,486,500.00 Danish Kroner

### Nanostructurers fysik og kemi

**Department of Physics**

- **Period:** 30/11/2001 → 29/11/2002
- **Number of participants:** 1
- **Project Manager, organisational:** Mørup, Steen (Intern)

**Financing sources**

- **Source:** Internal funding (public)
- **Name of research programme:** Grundforskningsfonden
- **Amount:** 15,684.00 Danish Kroner

### Nanostructured Materials

**Department of Physics**

- **Period:** 08/11/2001 → 30/06/2003
- **Number of participants:** 1
Project Manager, organisational:
Jiang, Jianzhong (Intern)

Financing sources
Source: Uddannelse. Statslige. Andre statslige
Name of research programme: Uddannelse. Statslige. Andre statslige
Amount: 75,000.00 Danish Kroner

Project

Synkronisering af tryk- og flowreguleringen i systemer af koblede nefroner
Department of Physics
Period: 05/11/2001 → 09/09/2003
Number of participants: 2
Project participant:
Sosnovtseva, Olga (Intern)
Project Manager, organisational:
Mosekilde, Erik (Intern)

Financing sources
Source: Forskningsrådene - SNF
Name of research programme: Forskningsrådene - STVF
Amount: 432,000.00 Danish Kroner

Project

Heterogeneous catalysis for asymmetric epoxidation reactions
Department of Physics
Period: 02/10/2001 → 30/09/2004
Number of participants: 1
Project ID: 20096
Project Manager, organisational:
Hagen, Anke (Ekstern)

Financing sources
Source: Forskningsrådene - STVF
Name of research programme: Forskningsrådene - STVF
Amount: 1,500,000.00 Danish Kroner

Project

Nanomagnetisme
Department of Physics
Number of participants: 6
Phd Student:
Frandsen, Cathrine (Intern)
Supervisor:
Lefmann, Kim (Ekstern)
Main Supervisor:
Mørup, Steen (Intern)
Examiner:
Skriver, Hans Lomholt (Intern)
McCammon, Catherine (Ekstern)
vander Zaag, Pieter J. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsstipendium
Project: PhD
Materialeudvikling og optimering på et kvantefysisk grundlag

Department of Physics
Period: 03/07/2001 → 31/10/2004
Number of participants: 1
Project ID: 20095
Project Manager, organisational: Vegge, Tejs (Ekstern)

Financing sources
Source: Forskningsrådene - Andre
Name of research programme: Forskningsrådene - Andre
Amount: 2,172,952.00 Danish Kroner
Project

Hydrogensamfund - ansøgning

Department of Physics
Period: 25/05/2001 → 15/11/2001
Number of participants: 1
Project ID: 20093
Project Manager, organisational: Chorkendorff, Ib (Ekstern)

Financing sources
Source: Forskningsrådene - STVF
Name of research programme: Forskningsrådene - STVF
Amount: 100,000.00 Danish Kroner
Project

EU Marie Curie Project, Benter

Department of Physics
Period: 15/05/2001 → 11/04/2003
Number of participants: 1
Project ID: 20092
Project Manager, organisational: Hagen, Anke (Ekstern)

Financing sources
Source: Forsk. EU - Rammeprogram
Name of research programme: Forsk. EU - Rammeprogram
Amount: 537,375.00 Danish Kroner
Project

Coherence and Adaptation in Populations with Parameter Distribution

Department of Physics
Period: 01/05/2001 → 19/08/2004
Number of participants: 6
Phd Student: de Monte, Silvia (Intern)
Supervisor: Giorgilli, Antonio (Ekstern)
Main Supervisor: Mosekilde, Erik (Intern)
Examiner: Bohr, Tomas (Intern)
Hakim, Vincent (Ekstern)
Hudson, John (Ekstern)

Financing sources
Source: Internal funding (public)
Modelling of Glucose-Clamp

Department of Physics
Period: 01/04/2001 → 02/02/2005
Number of participants: 7
Phd Student:
Groth, Andreas Velsing (Ekstern)
Supervisor:
Ingwersen, Steen Hvass (Ekstern)
Thomsen, Mikael S. (Ekstern)
Main Supervisor:
Mosekilde, Erik (Intern)
Examiner:
Knudsen, Carsten (Intern)
Heinemann, Lutz (Ekstern)
Sturis, Jeppe (Ekstern)

Financing sources
Source: Internal funding (public)

Physiology-Based Modelling in Drug Development

Department of Physics
Period: 01/04/2001 → 19/08/2004
Number of participants: 7
Phd Student:
Diderichsen, Paul Matthias (Intern)
Supervisor:
Colding-Jørgensen, Morten (Ekstern)
Main Supervisor:
Mosekilde, Erik (Intern)
Examiner:
Knudsen, Carsten (Intern)
Proks, Peter (Ekstern)
Rinzel, John (Ekstern)
J. Kirby, Brian (Ekstern)

Financing sources
Source: Internal funding (public)

Stationary Viscous Flows with Free Surface and Vortex Structures in Plasmas Flows

Department of Physics
Period: 01/03/2001 → 27/10/2004
Number of participants: 6
Phd Student:
Senchenko, Sergey (Intern)
Supervisor:
Rasmussen, Jens Juul (Intern)
Main Supervisor:
Bohr, Tomas (Intern)
Examiner:
Christiansen, Peter Leth (Intern)
Clanet, Christophe (Ekstern)  
Lautrup, Benny (Ekstern)

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: DTU, Samfinansiering  
Project: PhD

**Dynamik i koblede lange Josephson dioder**  
Department of Physics  
Period: 31/01/2001 → 12/12/2002  
Number of participants: 2  
Project participant:  
Mahaini, Carsten Ehssan (Intern)  
Project Manager, organisational:  
Mygind, Jesper (Intern)

**Financing sources**  
Source: Gaver, Private danske Fonde  
Name of research programme: Gaver, Private danske Fonde  
Amount: 30,000.00 Danish Kroner

**Hou Wei**  
Department of Physics  
Period: 30/01/2001 → 14/05/2003  
Number of participants: 2  
Project participant:  
Wei, Hou (Ekstern)  
Project Manager, organisational:  
Buchhave, Preben (Intern)

**Financing sources**  
Source: Forsk. Private danske - Andre  
Name of research programme: Forsk. Private danske - Andre  
Amount: 37,980.00 Danish Kroner

**Magnetiske nanokompositmaterialer**  
Department of Physics  
Period: 04/01/2001 → 25/02/2004  
Number of participants: 1  
Project ID: 20078  
Project Manager, organisational:  
Mørup, Steen (Ekstern)

**Financing sources**  
Source: Forskningsrådene - STVF  
Name of research programme: Forskningsrådene - STVF  
Amount: 558,000.00 Danish Kroner

**Magnetiske nanokompositmaterialer**  
Department of Physics  
Period: 04/01/2001 → 25/02/2004  
Number of participants: 1  
Project Manager, organisational:  
Mørup, Steen (Intern)
Financing sources
Source: Forskningsrådene - SNF
Name of research programme: Forskningsrådene - STVF
Amount: 558,000.00 Danish Kroner
Project

Nanomagnetisme
Department of Physics
Period: 04/01/2001 → 31/12/2005
Number of participants: 1
Project Manager, organisational:
Mørup, Steen (Intern)

Financing sources
Source: Forskningsrådene - STVF
Name of research programme: Forskningsrådene - STVF
Amount: 10,000,000.00 Danish Kroner
Project

Nanomagnetisme
Department of Physics
Risø National Laboratory for Sustainable Energy
Center for Nanoteknologi
University of Copenhagen
University of Iceland
The Open University
Virginia Commonwealth University
Uppsala University
Aarhus University
Period: 04/01/2001 → 31/03/2007
Number of participants: 10
Project ID: 20079
Project participant:
Lindelof, Poul Erik (Ekstern)
Lefmann, Kim (Intern)
Johnson, Erik (Intern)
Helgason, Örn (Ekstern)
Berry, Frank J. (Ekstern)
Carpenter, Everett (Ekstern)
Peter Svedlindh (Ekstern)
Gunnaugsson, Haraldur P. (Ekstern)
Weyer, Gerd (Ekstern)
Project Manager, organisational:
Mørup, Steen (Ekstern)

Financing sources
Source: Forskningsrådene - STVF
Name of research programme: Forskningsrådene - STVF
Amount: 3,039,000.00 Danish Kroner
Project

Apparaturbevilling
Department of Physics
Quantum description of enzyme function

Department of Physics
Period: 01/01/2001 → 23/03/2004
Number of participants: 6
Phd Student:
Hinnemann, Berit (Intern)
Supervisor:
Jacobsen, Karsten Wedel (Intern)
Main Supervisor:
Nørskov, Jens Kehlet (Intern)
Examiner:
Schietz, Jakob (Intern)
Stoltze, Per (Intern)
Trout, Bernhardt L. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-lønnet stipendie
Project: PhD

EU Marie Curie Project, Lopez

Department of Physics
Period: 25/10/2000 → 07/03/2002
Number of participants: 1
Project ID: 20070
Project Manager, organisational:
Nørskov, Jens Kehlet (Ekstern)

Financing sources
Source: Forsk. EU - Andre EU-midler
Name of research programme: Forsk. EU - Andre EU-midler
Amount: 501,475.00 Danish Kroner
Project:

Exchange - korrelationsfunktionaler i tæthedsfunktionalteori

Department of Physics
Period: 01/09/2000 → 01/12/2003
Number of participants: 5
Phd Student:
Bligaard, Thomas (Intern)
Main Supervisor:
Nørskov, Jens Kehlet (Intern)
Examiner:
Chorkendorff, Ib (Intern)
Clausen, Bjarne S. (Intern)
Hafner, Jürgen (Ekstern)

Financing sources
Dislokationkerners struktur og dynamik

Department of Physics
Period: 01/08/2000 → 26/02/2004
Number of participants: 6
Phd Student:
Frederiksen, Søren Lund (Intern)
Supervisor:
Schiøtz, Jakob (Intern)
Main Supervisor:
Jacobsen, Karsten Wedel (Intern)
Examiner:
Nørskov, Jens Kehlet (Intern)
Finnis, Michael William (Ekstern)
Leffers, Torben (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Grundforskningsfonden
Project: PhD

Magnetic Dynamics in Nanoparticles

Department of Physics
Period: 01/05/2000 → 26/11/2004
Number of participants: 7
Phd Student:
Klausen, Stine Nyborg (Intern)
Supervisor:
Clausen, Kurt Nørgaard (Intern)
Lefmann, Kim (Ekstern)
Main Supervisor:
Mørup, Steen (Intern)
Examiner:
Gerward, Leif (Intern)
Enderle, Mechthild (Ekstern)
McEwen, Keith Alistair (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut, samfinansiering
Project: PhD

Gæsteprofessor, Daniel Resasco

Department of Physics
Period: 12/04/2000 → 21/06/2001
Number of participants: 1
Project ID: 20043
Project Manager, organisational:
Chorkendorff, Ib (Ekstern)

Financing sources
Source: Forsk. Andre statslige danske - Forskerudd.kontoret
Name of research programme: Forsk. Andre statslige danske - Forskerudd.kontoret
Amount: 335,900.00 Danish Kroner
Project
Nanomechanics for metals and alloys

Department of Physics
Period: 05/04/2000 → 31/12/2004
Number of participants: 1
Project ID: 20041
Project Manager, organisational:
Jacobsen, Karsten Wedel (Ekstern)

Financing sources
Source: Forskningsrådene - STVF
Name of research programme: Forskningsrådene - STVF
Amount: 2,680,880.00 Danish Kroner

New design strategies for catalysts

Department of Physics
Period: 05/04/2000 → 31/12/2005
Number of participants: 1
Project ID: 20042
Project Manager, organisational:
Chorkendorff, Ib (Ekstern)

Financing sources
Source: Forskningsrådene - STVF
Name of research programme: Forskningsrådene - STVF
Amount: 4,440,000.00 Danish Kroner

Jesper Christiansen ph.d.-projekt

Department of Physics
Period: 01/04/2000 → 30/11/2003
Number of participants: 1
Project ID: 20040
Project Manager, organisational:
Jacobsen, Karsten Wedel (Ekstern)

Financing sources
Source: Uddannelse. Sektorforskning. Risø
Name of research programme: Uddannelse. Sektorforskning. Risø
Amount: 240,000.00 Danish Kroner

Populations of Dynamical Systems for Interacting Living Cells and Complex Systems

Department of Physics
Period: 01/04/2000 → 05/02/2003
Number of participants: 7
Phd Student:
D'Ovidio, Francesco (Intern)
Supervisor:
Porati, Alfredo (Ekstern)
Sørensen, Preben Graae (Ekstern)
Main Supervisor:
Mosekilde, Erik (Intern)
Examiner:
Hjorth, Poul G. (Intern)
Tass, Peter A. (Ekstern)
Westerhoff, Hans V. (Ekstern)
Financing sources  
Source: Internal funding (public)  
Name of research programme: Friplads  
Project: PhD  

Struktur og mekaniske egenskaber af nanokrystallinske materialer  
Department of Physics  
Period: 01/04/2000 → 01/12/2003  
Number of participants: 7  
Phd Student: Christiansen, Jesper (Intern)  
Supervisor: Jacobsen, Karsten Wedel (Intern)  
Leffers, Torben (Intern)  
Main Supervisor: Schiøtz, Jakob (Intern)  
Examiner: Nørskov, Jens Kehlet (Intern)  
Battiger, Jørgen (Intern)  
Devincre, Benoit (Ekstern)  

Financing sources  
Source: Internal funding (public)  
Name of research programme: Risø (Løn)  
Project: PhD  

Flavour Release from Model Systems - In Vitro and In Vivo Instrumental Measurements  
Department of Physics  
Period: 01/03/2000 → 28/05/2003  
Number of participants: 7  
Phd Student: Dinesen, Anders Reves (Intern)  
Supervisor: Linderoth, Søren (Intern)  
Pryds, Nini (Intern)  
Main Supervisor: Mørup, Steen (Intern)  
Examiner: Jacobsen, Claus Schelde (Intern)  
Pankhurst, Quentin Andrew (Ekstern)  
Rasmussen, Finn Berg (Ekstern)  

Financing sources  
Source: Internal funding (public)  
Name of research programme: Forskerakademiets Samfinansier  
Project: PhD  

Programmable phase optics for optical tweezers  
Department of Physics  
Period: 01/03/2000 → 06/10/2003  
Number of participants: 6  
Phd Student: Eriksen, René Lynge (Intern)  
Supervisor: Glückstad, Jesper (Intern)  
Main Supervisor: Skettrup, Torben (Intern)
Density functional theory used on biological systems
Department of Physics
Period: 01/02/2000 → 12/02/2004
Number of participants: 6
Phd Student: Rossmeisl, Jan (Intern)
Supervisor: Jacobsen, Karsten Wedel (Intern)
Main Supervisor: Nørskov, Jens Kehlet (Intern)
Examiner: Skriver, Hans Lomholt (Intern)
Pettersson, Lars G. M. (Ekstern)
Scheffler, Matthias (Ekstern)

Modelling of fast oscillations in katabolic beta-cells
Department of Physics
Period: 01/02/2000 → 02/02/2005
Number of participants: 8
Phd Student: Luciani, Dan Seriano (Intern)
Supervisor: Misler, Stanley (Ekstern)
Polonsky, Kenneth S. (Ekstern)
Sturis, Jeppe (Ekstern)
Main Supervisor: Mosekilde, Erik (Intern)
Examiner: Knudsen, Carsten (Intern)
Arkhammar, Per O. G. (Ekstern)
Krippeit-Drews, Peter (Ekstern)

Spin-polarised transport in semiconductors
Department of Physics
Period: 01/02/2000 → 02/12/2003
Number of participants: 8
Phd Student:
Bifurcations and Chaos in piecewise Smooth Dynamical Systems

Technical problems often lead to differential equations with piecewise smooth right-hand sides. Problems in mechanical engineering, for instance, violate the conditions of smoothness if they involve collisions, finite clearances, or stick-slip phenomena. Systems of this type can display a large variety of complicated bifurcation scenarios that still lack a detailed description. The purpose of this project is to study a range of new phenomena that can arise in piecewise-smooth dynamical systems, including new types of direct transitions to chaos, modified period-doubling, saddle-node and Hopf bifurcations, truncated bifurcation series, period-tripling and-quadrupling bifurcations, and multiple-choice bifurcations. Particular emphasis is given to the study of torus destruction in non-smooth systems. The practical significance of these phenomena will be demonstrated through a series of well-documented applications to switching power converters, to relay systems with and without hysteresis and time deadzones, and to different forms of pulse-width modulated control systems.

Graduate School in Nonlinear Science

The Center for Modelling, Nonlinear Dynamics and Irreversible Thermodynamics (MIDIT) at the Technical University of Denmark (DTU), the Department of Optics and Fluid Dynamics (OFD) at Risø National Laboratory (Risø), and the Center of Chaos and Turbulence Studies (CATS) at Copenhagen University (KU) conduct a Graduate School in Nonlinear Science. In collaboration with industry, this school provides a Danish Ph.D. program at the highest international level with the aim of preparing students to apply recent advances in Nonlinear Science to outstanding problems of science and technology and to strengthen international exchange of Ph.D. students. Over the past three decades, science has experienced a revolutionary shift in its fundamental paradigms. Primarily based on linear models through the 1960s, scientific research is now commonly motivated by nonlinear concepts, in which the whole is more than the sum of its parts, and the emergence of qualitatively new phenomena is anticipated and made welcome. The basic theme of modern Nonlinear Science is the interplay between chaos and coherent structures. Formerly deemed unworthy of the attention of a serious scientist, low order systems of nonlinear ordinary differential equations are now known to exhibit explosive behavior, leading to the emergence of strange attractors upon which phase space trajectories wander aimlessly until the end of time. Largely ignored as being far too difficult to solve analytically, nonlinear partial differential equations have been found to generate the emergence of solitary waves, which interact as new dynamic entities at higher levels of description. These new paradigms lead to significant advances in our understanding of a number of observed phenomena in physics, chemistry, and biology. From the theory, methods for constructive applications in the engineering sciences have been developed, using computer technology.
Marie Curie Training site
Ph. D. courses and research training through participation in projects and courses on: coherent structures and vortex dynamics, wave patterns, turbulence and chaos, nonlinear optics, lattices, superconduction, nanoelectronics, biomolecular dynamics, physiological control

CICT
Department of Informatics and Mathematical Modeling
Biophysics and Fluids
Department of Physics
University of Copenhagen
Novo Nordisk A/S

RISØ
Period: 01/01/2000 → 31/12/2002
Number of participants: 8
Project participant:
Scott, Alwyn C. (Intern)
Mosekilde, Erik (Intern)
Høgh Hansen, M. (Ekstern)
Colding-Jørgensen, M. (Ekstern)
Johansen, P. M. (Ekstern)
Rasmussen, J. Juul (Ekstern)
Graae Sørensen, P. (Ekstern)

Modellering, ikke-lineær Dynamik og irreversibel termodynamik (MIDIT)

Department of Informatics and Mathematical Modeling
Department of Mathematics
Department of Physics
Administration
Department of Chemistry
**Geometric knot theory with applications to proteins**

This project focuses on relations between the geometry of protein backbones and the geometry of framed space curves. This is done with the purpose of finding continuous models of protein backbones, such that protein structure and dynamics can be studied by methods of (global) differential geometry and infinite dimensional dynamical systems.

Department of Mathematics

Department of Physics

Period: 01/09/1999 → 31/08/2001
Number of participants: 2

Project participant:
Bohr, Henrik (Intern)

Project Manager, organisational:
Røgen, Peter (Intern)

**Financing sources**
Source: Unknown
Name of research programme: Ukendt
Amount: 360,000.00 Danish Kroner

**Reduktion af kvantefluktuationer ved brug af optiske x(2)-processer**

Department of Physics

Period: 01/09/1999 → 06/03/2003
Number of participants: 5

Phd Student:
Andersen, Ulrik Lund (Intern)
Main Supervisor:
Buchhave, Preben (Intern)
Examiner:
Tromborg, Bjarne (Intern)
Leuchs, Gerd (Ekstern)
Polzik, Eugene (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: DTU-lønnet stipendie
Project: PhD

**Struktur og elektriske egenskaber af molekyler ved overflader**

Department of Physics

Period: 01/09/1999 → 15/11/2002
Number of participants: 5

Phd Student:
Bollinger, Mikkel (Intern)
Main Supervisor:
Jacobsen, Karsten Wedel (Intern)
Examiner:
Schiøtz, Jakob (Intern)
Hyldgaard, Per (Ekstern)
Niemin, Risto (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-lønnet stipendie
Project: PhD

EUCAS 2001 Conference - Copenhagen
ELTEK - DTU er valgt som vært og arrangør af "European Conference on applied Superconductivity", Copenhagen 26.-30. august 2001, hvortil der kommer 800 - 1000 deltagere. Konferencen holdes på DTU efter indbydelse fra Rektor. Til forberedelse og gennemførelse af konference er der dannet projektkomité - se project staff og project partners

Department of Electric Power Engineering
Department of Physics
Department of Electrical Engineering
DIS Congress Service
Nordic Superconductor Technology
Period: 01/08/1999 → 01/11/2001
Number of participants: 13
Project participant:
Hald, Britta (Intern)
Herse, Erik (Intern)
Hvirgeltøft, Georg (Intern)
Jensen, Kim Høj (Intern)
Larsen, Esben (Intern)
Leisner, Torben (Intern)
Pedersen, Niels Falsig (Intern)
Træholt, Chresten (Intern)
Däumling (fratrådt), Manfred (Intern)
Mygind, Jesper (Intern)
Jacobsen, Claus Schelde (Intern)
Renouf, Sophie (Ekstern)
Project Manager, organisational:
Tøennesen, Ole (Intern)

Financing sources
Source: Unknown
Name of research programme: Ukendt
Amount: 3,000,000.00 Danish Kroner
Project

Parallel Screening of Alloy Model Catalysts - a Methodological Approach
Department of Physics
Period: 01/08/1999 → 17/07/2003
Number of participants: 5
Phd Student:
Jørgensen, Jan Hoffmann (Intern)
Main Supervisor:
Chorkendorff, Ib (Intern)
Examiner:
Nielsen, Jane Hvolbæk (Intern)
Dahl, Søren (Ekstern)
Jugnet, Yvette (Ekstern)

Financing sources
ELKRAFT

Department of Physics
Period: 01/07/1999 → 22/03/2002
Number of participants: 1
Project ID: 20033
Project Manager, organisational:
Chorkendorff, Ib (Ekstern)

Financing sources
Source: Gaver, Private danske Andre private
Name of research programme: Gaver, Private danske Andre private
Amount: 1,500,000.00 Danish Kroner

Avancerede lasere med selektbar bølgelængde

Department of Physics
Period: 01/06/1999 → 28/06/2002
Number of participants: 7
Phd Student:
Jensen, Ole Bjarlin (Intern)
Supervisor:
Balle-Petersen, Olav (Ekstern)
Bruun-Larsen, Morten (Ekstern)
Main Supervisor:
Skettrup, Torben (Intern)
Examiner:
Buchhave, Preben (Intern)
Laurell, Fredrik (Ekstern)
Lindvold, Lars René (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Erhvervsforskerordningen
Project: PhD

Vortex flows with a free surface and random matrix theory and acoustic resonances

Department of Physics
Period: 01/06/1999 → 16/10/2002
Number of participants: 6
Phd Student:
Andersen, Anders Peter (Intern)
Supervisor:
Rasmussen, Jens Juul (Intern)
Main Supervisor:
Bohr, Tomas (Intern)
Examiner:
Sørensen, Jens Nørkær (Intern)
Lundgren, Thomas S. (Ekstern)
Wang, Jane (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut, samfinansiering
Project: PhD
Mechanical properties of materials
The aim of the project is to understand the mechanical properties of materials, in particular metals and alloys, by studying the atomic structure using computer simulations. The simulations are mostly based on the effective medium theory. The study focusses on crystal defects (in particular dislocations, cracks, grain boundaries and surfaces) and their mutual interactions. It includes both studies of idealized geometries such as a single crack near a grain boundary, and more realistic geometries such as nanocrystalline metals.

Department of Physics
Risø National Laboratory for Sustainable Energy
Period: 01/05/1999 → …
Number of participants: 6
Project participant:
Jacobsen, Karsten Wedel (Intern)
Vegge, Tejs (Intern)
Leffers, Torben (Intern)
Pedersen, Ole Bøcker (Intern)
Bilde-Sørensen, Jørgen (Intern)

Kaotisk synkronisering i biologiske systemer
Department of Physics
Period: 01/03/1999 → 01/12/2000
Number of participants: 2
Phd Student:
Andersen, Morten Dines (Intern)
Main Supervisor:
Mosekilde, Erik (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-lønnet stipendie
Project: PhD

Magnetfeltsegenskaber af superledere
Department of Physics
Period: 01/02/1999 → 20/05/2003
Number of participants: 7
Phd Student:
Abrahamsen, Asger Bech (Intern)
Supervisor:
Andersen, Niels Hessel (Intern)
Hansen, Jørn Otto Bindslev (Ekstern)
Main Supervisor:
Jacobsen, Claus Schelde (Intern)
Examiner:
Mygind, Jesper (Intern)
Hedegård, Per (Ekstern)
Mesot, Joël (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskerakademiets Samfinansier
Project: PhD
**Biomedical sensors**

At Research Center COM we have entered into a collaboration with other DTU institutions (namely Institute of Physics and IMM) and Forskningscenter Risø, concerning biomedical optics (BIOP). The BIOP initiative covers four focus areas. At COM we are primarily involved in the development of optical coherence tomography (OCT) systems, and over the past year, we have in collaboration with Forskningscenter Risø developed a theoretical/numerical model describing the noise-properties of practical OCT systems. In addition to this model, which has been used in the design of next generation OCT systems, detailed modelling of light propagation in random media (living tissue such as skin or eyes) has been performed. Results of this work have been presented at international conferences such as Conference on Optical Tomography and Spectroscopy of Tissue, San Jose, CA. Another key activity for Research Center COM concerning the BIOP collaboration has been the initial investigations of photonic crystal fibres (PCFs) in sensors. Here we make use of the fact that the PCFs contain micron wide holes and provide the possibility for guiding light in these. Hereby, an attractive alternative to evanescent field waveguides becomes possible, and at COM we have applied our detailed numerical tools in describing the waveguiding properties of such new sensor waveguides presented at the International Conference LIGHT FOR LIFE 99 in Cancun, Mexico.

**Fibers & Nonlinear Optics**

Department of Photonics Engineering

Rise National Laboratory for Sustainable Energy

Department of Physics

Department of Informatics and Mathematical Modeling

**Period:** 01/01/1999 → …

**Number of participants:** 5

**Project participant:**

Tycho, Andreas (Intern)

Buckhave, Preben (Ekstern)

Ersbøll, Bjarne (Ekstern)

Project Manager, organisational:

Bjarklev, Anders Overgaard (Intern)

Petersen, Paul Michael (Ekstern)

**Financing sources**

**Source:** Unknown

**Name of research programme:** Ukendt

**Amount:** 0.00 Danish Kroner

**Project**

**Graduate School in Nonlinear Science**

Projectno. 7317 Educational project aimed at PhD students Collaboration with Department of Optics and Fluid Dynamics, Rise National Laboratory, Center of Chaos and Turbulence Studies, Niels Bohr Institute, University of Copenhagen

Department of Informatics and Mathematical Modeling

Department of Physics

University of Copenhagen

Novo Nordisk A/S

**Forskningscenter Risø**

**Period:** 01/01/1999 → 31/12/1999

**Number of participants:** 8

**Project participant:**

Scott, Alwyn C. (Intern)

Jensen, M. Høgh (Ekstern)

Colding-Jørgensen, M. (Ekstern)

Johansen, Per Michael (Intern)

Rasmussen, Jens Juul (Intern)

Mosiekide, Erik (Intern)

Sørensen, P. G. (Ekstern)

Project Manager, organisational:

Christiansen, Peter Leth (Intern)
Instabilities in Chemical Reaction-Diffusion Systems with Flow

Chemical reaction-diffusion systems can display instabilities of the Hopf as well as of the Turing type. The Hopf instability is associated with the onset of spatially uniform oscillations in time whereas the Turing instability gives rise to the growth of stationary spatial patterns with a characteristic wavelength determined by the reaction and diffusion rates. The condition for the Turing instability to arise before the Hopf instability is usually that the diffusion constants of the basic reagents are very different. The purpose of the present study is to investigate the instabilities that can occur in a reaction-diffusion system with a uniform flow of the reactants. In this case, which clearly is relevant for many industrial processes, one has to distinguish between convective and absolute instabilities. The Galilean invariance of the system is broken by the presence of an inlet position for the reactor, and as a result, in the convectively unstable state one can observe various types of noise sustained patterns as well as stationary structures, even in the case of equal diffusion constants. Project members: Morten Bache and Peter Andresén, DTU; Guy Dewel and Pierre Borckmans, Free University of Brussels; Sergey Kuznetsov, Dept. of Physics, Saratov.

Development of Intracavity optical parametric oscillator

Department of Physics
Number of participants: 5
Phd Student: Abitan, Haim (Intern)
Main Supervisor: Buchhave, Preben (Intern)
Examiner: Skettrup, Torben (Intern)
Laurell, Fredrik (Ekstern)
Pedersen, Christian (Ekstern)

Development of a high temperature SQUID gradiometer for biomedical applications

Department of Physics
Period: 01/10/1998 → 26/03/2002
Number of participants: 5
Phd Student: Petersen, Peter Rasmus Ebsen (Intern)
Supervisor: Hansen, Jern Otto Bindslev (Ekstern)
Main Supervisor: Jacobsen, Claus Schelde (Intern)
Examiner: Mygind, Jesper (Intern)
Seidel, Paul (Ekstern)

Financing sources
Source: Internal funding (public)
Magnetic scanning of peripheral nerve activity - A new tool in clinical neurophysiology

Department of Physics
Period: 01/10/1998 → 14/06/2002
Number of participants: 9
Phd Student:
Nordahn, Morten Agerbæk (Intern)
Supervisor:
Burghoff, Martin (Ekstern)
Hansen, Jern Otto Bindslev (Ekstern)
Holst, Thorsten (Ekstern)
Krarup, Christian (Ekstern)
Main Supervisor:
Jacobsen, Claus Schelde (Intern)
Examiner:
Jensen, Jørgen Arendt (Intern)
Koch, Hans (Ekstern)
Nenonen, Jukka (Ekstern)

Financing sources
Source: Internal funding (public)

Tejs Vegge ph.d.-projekt

Department of Physics
Period: 01/10/1998 → 12/02/2002
Number of participants: 1
Project ID: 20023
Project Manager, organisational:
Jacobsen, Karsten Wedel (Ekstern)

Financing sources
Source: Uddannelse. Sektorforskning. Risø
Name of research programme: Uddannelse. Sektorforskning. Risø
Amount: 242,800.00 Danish Kroner

Waveguide Holography
Waveguide holography is an improved technique for storing holographic information. In this project the feasibility of storing information in waveguide holograms followed by reconstructing with white light is examined.

Department of Physics
Xiamen University
Number of participants: 2
Project participant:
Lai, Hongkai (Ekstern)
Project Manager, organisational:
Dalsgaard, Erik (Intern)

Center for Atomic-scale Materials Physics (CAMP)
The general theme for the research in CAMP is the study of metallic nano-structures and their properties by a closely coupled experimental and theoretical approach. In the present report the research is organized under three main headings: 1. Nano-structures, focused on an understanding of structural, mechanical, and electrical properties of nano-structures. 2. Surface alloys and surface chemical properties, focused on the understanding, design, and synthesis of
surfaces and the possibility of modifying and controlling their chemical reactivity. 3. Biomolecules, focused on the understanding of the structure and interactions within proteins, their enzymatic function, and their interactions with solid surfaces.

Department of Physics
Aarhus University
Period: 01/09/1998 → 31/12/2005
Number of participants: 12
Project ID: 20018
Project participant:
Jacobsen, Karsten Wedel (Intern)
Skriver, Hans Lomholt (Intern)
Chorkendorff, Ib (Intern)
Schietz, Jakob (Intern)
Horch, Sebastian (Intern)
Nielsen, Jane Hvolbæk (Intern)
Quaade, Ulrich (Intern)
Besenbacher, Flemming (Ekstern)
Stensgaard, Ivan (Ekstern)
Lægsgaard, Erik (Ekstern)
Hammer, Bjørk (Ekstern)
Project Manager, organisational:
Nørskov, Jens Kehlet (Ekstern)

Financing sources
Source: Forsk. Andre statslige danske - Grundforskn.fonden
Name of research programme: Forsk. Andre statslige danske - Grundforskn.fonden
Amount: 28,843,170.00 Danish Kroner
Project

Defektdynamik på atomar skala
Department of Physics
Period: 01/09/1998 → 03/12/2001
Number of participants: 5
Phd Student:
Vegge, Tejs (Intern)
Main Supervisor:
Jacobsen, Karsten Wedel (Intern)
Examiner:
Nørskov, Jens Kehlet (Intern)
Gumbsch, Peter (Ekstern)
Wahnström, Göran (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Risø (Løn)
Project: PhD

Dynamikken af hukommelses oplagring, overførsel og genkaldelse i komplekse neurale systemer
Department of Physics
Period: 01/09/1998 → 06/05/2002
Number of participants: 5
Phd Student:
Nielsen, Bjørn Gilbert (Intern)
Main Supervisor:
Cotterill, Rodney M J (Intern)
Examiner:
Bohr, Henrik (Intern)
Carpenter, Roger (Ekstern)
Franser, Erik (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Ansat eksternt
Project: PhD

**Støjmekanismer og ulineære effekter i nanostrukturer med henblik på anvendelser i fremtidig rumligt begrænset elektronik**

Department of Physics
Number of participants: 6
Phd Student:
Manscher, Martin (Intern)
Supervisor:
Samuelsen, Mogens Rugholm (Intern)
Main Supervisor:
Mygind, Jesper (Intern)
Examiner:
Jacobsen, Claus Schelde (Intern)
Haviland, David B. (Ekstern)
Zorin, Alexander B. (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: DTU-lønnet stipendie
Project: PhD

**Spin-polarised transport in ferromagnet/semiconductor heterostructure**
A study of injection and precession effects for spin-polarised carriers. The project aims at the development of spin-FETs (Field Effect Transistors) consisting of ferromagnet/semiconductor/ferromagnet heterostructures (eg Fe/GaAs-GaAlAs/Fe or Fe-Ni/InAs-InGaAs/Fe-Ni). Collaboration with The Oersted Lab (NBI), Danish Institute of Fundamental Metrology and NTT Basic Research Labs, Atsugi, Japan.

Department of Physics
Period: 01/08/1998 → …
Number of participants: 4
Project participant:
Kutchinsky, Jonatan (Intern)
Taboryski, Rafael J. (Intern)
Skov, Johannes (Intern)
Project Manager, organisational:
Hansen, Jern Bindslev (Ekstern)

**Financing sources**
Source: Unknown
Name of research programme: Ukendt
Amount: 250,000.00 Danish Kroner
Source: Unknown
Name of research programme: Ukendt
Amount: 50,000.00 Danish Kroner
Source: Unknown
Name of research programme: Ukendt
Amount: 112,000.00 Danish Kroner

**The structure and formation of sand-ripple patterns.**
We study the structure and formation of sand-ripple patterns under oscillating water both experimentally (at the Niels Bohr Institute) and theoretically.

Department of Physics
The structure of the circular hydraulic jump
We study the formation and structure of the circular hydraulic jump in various fluids. We are especially interested in the "polygonal" states that we discovered in 1998 (Nature 392, 707).

Department of Physics
Clive Ellegaard
Vakhtang Putkaradze
Shinya Watanabe

Kohærente strukturer og transport i driftsbølge-plasmaturbulens
Department of Physics
Period: 01/05/1998 → 18/10/2002
Number of participants: 7
Phd Student:
Korsholm, Søren Bang (Intern)
Supervisor:
Michelsen, Poul (Intern)
Rasmussen, Jens Juul (Intern)
Main Supervisor:
Mosekilde, Erik (Intern)
Examiner:
Bohr, Tomas (Intern)
Lashmore-Davies, C. N. (Ekstern)
Rypdal, Kristoffer (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskerakademiets Samfinansier
Project: PhD

Frequency multiplexed coherent light source
EU LTR Project under 4th Framework ESPRIT Programme Diode-pumped solid-state lasers, optical parametric oscillators, frequency multiplexed photorefractive holographic data storage, periodically poled, wide band KTP second harmonic generation, quasi phase matching.

Department of Physics
Period: 10/04/1998 → 01/08/1999
Number of participants: 1
Project Manager, organisational:
Buchhave, Preben (Intern)
Mikrokinetisk modellering af katalysatorer baseret på legeringer

Department of Physics
Period: 01/02/1998 → 30/07/2001
Number of participants: 7
Phd Student:
Christoffersen, Ebbe (Intern)
Supervisor:
Chorkendorff, Ib (Intern)
Stoltze, Per (Intern)
Main Supervisor:
Nørskov, Jens Kehlet (Intern)
Examiner:
Nielsen, Jane Hvolbæk (Intern)
Clausen, Bjerne S. (Intern)
Kramer, Jan Gert (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Centerfinansieret
Project: PhD

Strukturelle egenskaber af superledende BSCCO/Ag bånd under afkøling

Department of Physics
Period: 01/02/1998 → 18/09/2001
Number of participants: 7
Phd Student:
Egeberg, Lotte Gottschalck (Intern)
Supervisor:
Hansen, Jørn Otto Bindslev (Ekstern)
Poulsen, Henning Friis (Intern)
Main Supervisor:
Jacobsen, Claus Schelde (Intern)
Examiner:
Gerward, Leif (Intern)
Majelski, Peter (Ekstern)
Tholen, Anders Ragnar (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Risø (Løn)
Project: PhD

Teoretisk modellering af nanotribologiske fænomener

Department of Physics
Period: 01/02/1998 → 03/12/2001
Number of participants: 5
Phd Student:
Bahn, Sune Rastad (Intern)
Main Supervisor:
Jacobsen, Karsten Wedel (Intern)
Examiner:
Schiøtz, Jakob (Intern)
Puska, Martti Juhani (Ekstern)
Ruitenbeek, Jan van (Ekstern)

Financing sources
**Transition metal sulfides as catalysis**

Department of Physics  
Period: 01/02/1998 → 02/04/2002  
Number of participants: 6  
Phd Student: Bengaard, Hanne Skov (Intern)  
Supervisor: Rostrup-Nielsen, Jens (Intern)  
Main Supervisor: Nørskov, Jens Kehlet (Intern)  
Examiner: Jacobsen, Karsten Wedel (Intern)  
Lundqvist, Bengt I. (Ekstern)  
Schlögl, Robert (Ekstern)

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: DTU-lønnet stipendie  
Project: PhD

**Undersøgelser af potentielle legeringskatalysatorer ved brug af supersoniske molekylestråler**

Department of Physics  
Period: 01/02/1998 → 26/09/2001  
Number of participants: 5  
Phd Student: Egeberg, Rasmus (Intern)  
Main Supervisor: Chorkendorff, Ib (Intern)  
Examiner: Skriver, Hans Lomholt (Intern)  
Besenbacher, Flemming (Intern)  
Goodman, Wayne D. (Ekstern)

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: DTU-lønnet stipendie  
Project: PhD

**Interdisciplinary Research Center for Catalysis (ICAT)**

Department of Physics  
Period: 15/01/1998 → 23/12/2003  
Number of participants: 1  
Project ID: 20013  
Project Manager, organisational: Chorkendorff, lb (Ekstern)

**Financing sources**  
Source: Program. Andre statslige danske - IKT  
Name of research programme: Program. Andre statslige danske - IKT  
Amount: 8,168,664.00 Danish Kroner  
Project

**Cavitation research using microspheres as nuclei**

Der udføres målinger af vands trækstyrke efter at det er renset for partikler og derefter tilsat kendte microspheres af specificeret størrelse. Måleresultaterne relateres til K.A.Mørch’s model for dannelse af kavitations-kerner. Eksperimentelt
arbejde er udført som eksamensprojekt i Obernach i 1998.

Department of Physics
Institut for termisk energi, vannkraft, NTH
Technische Universität München
Period: 01/01/1998 → …
Number of participants: 3
Project participant:
Kjeldsen, Morten (Ekstern)
Project Manager, organisational:
Mørch, Knud Aage (Intern)
Keller, Andreas (Ekstern)

Compressibility and high-pressure phases of metal oxides

There is a current interest in the derivation of the parameters that define the equation of state (EOS) of polymorphs that are unstable under room conditions [1]. We report the results of a combined experimental and theoretical investigation on the stability and the volume behavior under hydrostatic pressure of the rocksalt (B 1) phase of ZnO. Synchrotron-radiation x-ray powder-diffraction data were obtained from 0 to 30 GPa. Static simulations of the ZnO B 1 phase were performed using the ab initio perturbed ion method and the local and nonlocal approximations to the density-functional theory. Nanostructured ZnO will be compared with bulk material.

Department of Physics
Universidad de Oviedo
Period: 01/01/1998 → …
Number of participants: 4
Project participant:
Jiang, Jianzhong (Intern)
Olsen, J. Staun (Ekstern)
Recio, J.M. (Ekstern)
Project Manager, organisational:
Gerward, Leif (Intern)

Financing sources
Source: Unknown
Name of research programme: Ukendt
Amount: 1,110.00 Danish Kroner
Source: Unknown
Name of research programme: Ukendt
Amount: 1,120.00 Danish Kroner

Compressibility of nanostructured materials prepared by mechanical milling

High-energy ball milling is widely used for the preparation of materials that are far from equilibrium, e.g. nanostructured, amorphous, and supersaturated alloys and ceramics. Compressibility of nanostructured Fe-Cu materials has been investigated by in-situ high pressure x-ray diffraction using synchrotron radiation. It is found that the bulk modulus of both fcc-Cu and bcc-Fe phases decreases with decreasing grain size. In contrast, small amounts of dopants, i.e. Fe in fcc-Cu and Cu in bcc-Fe, increase the bulk modulus of the metal matrix. The unstable ferromagnetic fcc-FeCu solid solution prepared by mechanical alloying has a bulk modulus of about 85 GPa which is much smaller than the corresponding values for bulk fcc-Cu and bcc-Fe.

Department of Physics
University of Copenhagen
Period: 01/01/1998 → 31/12/2002
Number of participants: 4
Project participant:
Jiang, Jianzhong (Intern)
Mørup, Steen (Intern)
Olsen, J. Staun (Ekstern)
High-pressure diffraction studies of spinel oxides
The phase transition and compressibility of the spinel oxides NiMn2O4 and ZnMn2O4 have been investigated at ambient temperature up to 60 GPa. The phase transition is attributed to the Jahn-Teller type distortion caused by Mn3+ ions acting as tetrahedral Jahn-Teller ions.

Department of Physics
University of Copenhagen
Period: 01/01/1998 → …
Number of participants: 4
Project participant:
Jiang, Jianzhong (Intern)
Olsen, J. Staun (Ekstern)
Waskowska, A. (Ekstern)
Project Manager, organisational:
Gerward, Leif (Intern)

Financing sources
Source: Unknown
Name of research programme: Ukendt
Amount: 1,110.00 Danish Kroner

High-pressure X-ray diffraction study of nitrides
Preliminary experiments were performed on moisture sensitive terbium nitride (TbN) in a diamond anvil pressure cell up to 50 GPa at ambient temperature.

Department of Physics
University of Copenhagen
Aarhus University
Period: 01/01/1998 → …
Number of participants: 4
Project participant:
Jiang, Jianzhong (Intern)
Olsen, J. Staun (Ekstern)
Jørgensen, J.E. (Ekstern)
Project Manager, organisational:
Gerward, Leif (Intern)

Financing sources
Source: Unknown
Name of research programme: Ukendt
Amount: 1,110.00 Danish Kroner

Source: Unknown
Name of research programme: Ukendt
Amount: 1,120.00 Danish Kroner

Project
Phase diagram of TiO₂

Experimental and theoretical calculations recently indicated that TiO₂ could have a series of high-pressure phases with a hardness possibly approaching that of a diamond. The high-pressure, high-temperature phase equilibria have been studied [1] with special emphasis on the rutile alpha-PbO₂ type phases. It is found that the phase boundary, when plotted in a pressure - temperature diagram, changes from negative to positive slope with increasing temperature at about 6 GPa and 850 °C. For nanophase material, the phase boundary is shifted towards lower pressure. The room-temperature bulk moduli are 210, 258 and 290 GPa for rutile, the alpha-PbO₂ type phase and the baddeleyite type phase, respectively.

Department of Physics

University of Copenhagen
Period: 01/01/1998 → 31/12/2000
Number of participants: 3
Project participant:
Jiang, Jianzhong (Intern)
Olsen, J. Staun (Ekstern)
Project Manager, organisational:
Gerward, Leif (Intern)

Financing sources
Source: Unknown
Name of research programme: Ukendt
Amount: 1,110.00 Danish Kroner
Source: Unknown
Name of research programme: Ukendt
Amount: 1,120.00 Danish Kroner

Pressure effect in the Hg-based superconductors

Energy-dispersive synchrotron x-ray diffraction studies [3] were performed on powder samples of Hg 1212 and Hg 1223 in a diamond-anvil cell at pressure up to 30 GPa, in order to study changes under pressure in these compounds, because pressure dependence might supply information regarding the mechanism of high-temperature superconductivity. High compressability of these compounds was observed and was suggested to correspond to a pressure-induced ordering along the c-axis. The structured importance of an Ba ion shift was demonstrated, and the effect to result from Ba-O gamma attraction. We suggest that the buffer layer plays an important role in increasing Tc by "fine tuning" the Ba position. A crucial role in enabling the Ba shift is played by the HgO gamma layer at high pressure.

Department of Physics

University of Copenhagen
Period: 01/01/1998 → 31/12/1999
Number of participants: 2
Project participant:
Olsen, J. Staun (Ekstern)
Project Manager, organisational:
Gerward, Leif (Intern)

Financing sources
Source: Unknown
Name of research programme: Ukendt
Amount: 1,120.00 Danish Kroner

Synthesis of Nanostructured Materials by High-Energy Ball Milling

The field of nanostructured materials is in a rapid development in many disciplines, e.g. condensed matter physics and materials science. Several techniques have been applied for sample preparation, for example, gas condensation, sputtering, electrodeposition, and thermochemical methods. One of the methods that has received significant attention is mechanical attrition: the high-energy ball milling of single or multicomponent powders. In this year, we successfully synthesised nanometer-sized ZnFe₂O₄, NiFe₂O₄, CuFe₂O₄, nanoalloying in Fe₂O₃-SnO₂, Fe-Cu and mechanochemical reactions in Fe-S.

Department of Physics
Department of Chemistry
Density functional theory calculations for surface reactions

Department of Physics
Period: 01/12/1997 → 30/11/2001
Number of participants: 5
Phd Student:
Logadottir, Ashildur (Intern)
Main Supervisor:
Nørskov, Jens Kehlet (Intern)
Examiner:
Schiøtz, Jakob (Intern)
Billing, Gert Due (Ekstern)
Ertl, Gerhard (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Centerfinansieret
Project: PhD

High-pressure behaviour of nanostructured materials

Nanostructured materials, consisting of small crystallites of diameters 1-100 nm, often have novel physical and chemical properties, different from those observed in bulk materials. The aim of the project is to understand the effects of crystallite size on solid-solid phase transitions in nanostructured materials by performing in-situ high pressure synchrotron x-ray diffraction measurements for a wide range of nanostructured materials. The research will address and answer a number of important questions related to the understanding of first order solid-solid phase transitions induced by pressure.
Department of Physics

Department of Chemistry

University of Copenhagen

Period: 01/10/1997 → …

Number of participants: 5

Project participant:
Jiang, Jianzhong (Intern)
Mørup, Steen (Intern)
Nielsen, Kurt (Intern)
Olsen, J. Staun (Ekstern)

Project Manager, organisational:
Gerward, Leif (Intern)

**Financing sources**

Source: Unknown

Name of research programme: Ukendt

Amount: 3,000,000.00 Danish Kroner

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**Højfrekvens- og støjegenskaber af nano-tunnelstrukturer**

Department of Physics

Period: 01/10/1997 → 27/03/2002

Number of participants: 6

Phd Student:
Ejrnæs, Mikkel (Intern)

Supervisor:
Jensen, Hans Dalsgaard (Ekstern)
Samuelsen, Mogens Rugholm (Intern)

Main Supervisor:
Mygind, Jesper (Intern)

Examiner:
Jacobsen, Claus Schelde (Intern)
Zorin, Alexander B. (Ekstern)

**Financing sources**

Source: Internal funding (public)

Name of research programme: DTU-Su Stipendium, Eksperiment

Project: PhD

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**Syntese og lavtemperatur karakterisering af nye materialekombinationer til fremstilling af hybride elektroniske komponenter**

Department of Physics

Period: 01/10/1997 → 18/09/2001

Number of participants: 7

Phd Student:
Kutchinsky, Jonatan (Intern)

Supervisor:
Hansen, Jørn Otto Bindslev (Ekstern)
Taboryski, Rafael J. (Intern)

Main Supervisor:
Jacobsen, Claus Schelde (Intern)

Examiner:
Mygind, Jesper (Intern)
Esteve, Daniel (Ekstern)
Strunk, Christoph (Ekstern)

**Financing sources**
Synthesis and low temperature characterisation of new material combinations for fabrication of hybrid electronic devices

Nanostructures based on new material combinations of superconductors, semiconductors and ferromagnetic materials are studied to achieve a better fundamental understanding of these materials, and to investigate the possibilities for new types of hybrid electronic devices.

Department of Physics
Period: 01/10/1997 → ...
Number of participants: 9
Project participant:
Kutchinsky, Jonatan (Intern)
Hansen, Jern Bindslev (Ekstern)
Skov, Johannes (Intern)
Rasmussen, Inge (Intern)
Jacobsen, Claus Schelde (Intern)
Lindelof, Poul Erik (Ekstern)
Sørensen, Claus B. (Ekstern)
Kuhn, Oliver (Ekstern)
Project Manager, organisational:
Taboryski, Rafael J. (Intern)

Financing sources
Source: Unknown
Name of research programme: Ukendt
Amount: 1,000,000.00 Danish Kroner

Optisk kohærenstomografi med ultrahej opløsning til non-invasiv medicinsk diagnostik

Department of Physics
Period: 01/03/1997 → 30/07/2001
Number of participants: 6
Phd Student:
Thrane, Lars (Intern)
Supervisor:
Hanson, Steen Grüner (Intern)
Main Supervisor:
Skettrup, Torben (Intern)
Examiner:
Bjarklev, Anders Overgaard (Intern)
Birngruber, Reginald (Ekstern)
Hitzenberger, Christoph K. (Ekstern)
Chaotic Synchronization and Riddled Basins of Attraction

The topic of chaotic synchronization is presently at the forefront of much research in the mathematically oriented dynamical systems theory as well as in more applied fields of secure communication and dynamical systems monitoring. The aim of the present project is to study the appearance of riddled basins of attraction and on-off intermittency for systems of coupled one- and two-dimensional maps. Special emphasis is given to the role of the so-called absorbing area in accounting for the distinction between local and global riddling and between hysteretic and non-hysteretic blowout.

Department of Physics

National Academy of Sciences of Ukraine
Period: 01/02/1997 → …
Number of participants: 2
Project participant:
Maistrenko, Yuri (Ekstern)
Project Manager, organisational:
Mosekilde, Erik (Intern)

Nonvolatile Optical Storage - Application to Lanthanum Gallium Silicate

Department of Physics
Period: 01/02/1997 → 22/05/2000
Number of participants: 5
Phd Student:
Nikolajsen, Thomas (Intern)
Supervisor:
Johansen, Per Michael (Intern)
Main Supervisor:
Skettrup, Torben (Intern)
Examiner:
Bozhevolnyi, Sergey I. (Intern)
Keiding, Søren Rud (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskerakademiets Samfinansier
Project: PhD

Decommissioning of Research Reactors

The project centers around the DR2 research reactor which was closed down in 1975, and the aim of the project is to investigate what further decommissioning steps are to be taken with the reactor. In addition cooperation in the field of research reactor decommissioning with Latvia and Poland have been investigated under the Danish sector programme, involving the countries around the Baltic Sea and run by the Danish Emergency Management Agency. As part of this work a report on the technical problems connected to the decommissioning of research reactors has been prepared. Also a contract has been signed with the International Atomic Energy Agency on decommissioning studies. A working group has been formed at Rise that will be responsible for the future work on DR2.

Department of Physics
Period: 15/01/1997 → 31/12/1998
Number of participants: 1
Project Manager, organisational:
Ølgaard, Povl Lebeck (Intern)

Dynamics of Product Formation in Myeloperoxidose-H2O2 Chloride System

Research on the chemistry of myeloperoxidose (MP) is proposed, leading to design of an effector of dynamic drug delivery (automatically recurrent delivery of therapeutic activity in synchrony with the need to counteract a pathological process) in subsequent work. Such dynamic drug delivery, either of MP or of some species released in consequence of MP's activity,
could maximize therapeutic effectiveness while reducing drug side effects. Simulations show prerequisite periodic reactions can be catalyzed by MP, an effector of periodicity. The system includes MP-H2O2-C1 and tyrosine reactions. It will be modulated by O2, CO2, and taurine. A combined experimental and computational approach will lead to the goal of finding, analyzing and modeling domains of temporal periodicity in the concentration of compounds significantly contributing to the biochemistry of the MP chlorinating system in an in vitro environment approximating the leukocytric milieu. Regulation of the MP-H2O2-C1 system by the aforementioned species will be studied in the physiologically important range of pH (4.5 to 8.0) and temperature (298 to 318 K). Structure of intermediates and products will be analyzed. Collaborative theoretical modeling of MP structure-property relationships will be conducted. Required instrument adaptations and method development will be carried out. A stopped-flow spectrometer will be upgraded with modern electronics. Near infrared measurements will be developed to analyze species. NIR methods can later be used for in vito monitoring of dynamic drug delivery. In subsequent work, periodic interaction will be elicited from cell cultured and subsequently tissues of mammals in steady contact with the drug delivery device developed as a consequence of this work.

Department of Physics
University of Illinois
Period: 01/01/1997 → ...
Number of participants: 3
Project participant:
Kirkor, Ewa S. (Ekstern)
Project Manager, organisational:
Bohr, Henrik (Intern)
Scheeline, Alexander (Ekstern)

**Dynamics of the magnetization in antiferromagnetic nanoparticles**
Ultrafine particles of hematite (alpha-Fe2O3) with an average size of about 15 nm have been prepared by controlled heating of ferric nitrate. The fluctuations of the sublattice magnetization directions have been studied by combining Mossbauer spectroscopy and magnetization measurements. Two different modes of superparamagnetic fluctuation of the particle moment have been observed. This shows that the behavior of these antiferromagnetic hematite particles are more complicated than the usual ferri- and ferromagnetic particles which exhibit only one such mode. The particles have also been studied by neutron scattering, and for the first time it has been shown that one can obtain information about magnetic fluctuations in nanoparticles by use of this technique. This was done by inelastic neutron scattering on an antiferromagnetic reflection. Even smaller hematite particles have now been prepared and the study of these particles is currently in progress. A similar study on nickel oxide (NiO) nanoparticles are now in progress.

Department of Physics
Risø National Laboratory for Sustainable Energy
Period: 01/01/1997 → 31/12/1998
Number of participants: 6
Project participant:
Bødker, Franz (Intern)
Hansen, Mikkel Fougt (Intern)
Lefmann, Kim (Intern)
Clausen, Kurt Nergaard (Intern)
Lindgård, Per-Anker (Intern)
Project Manager, organisational:
Marup, Steen (Intern)

**Financing sources**
Source: Unknown
Name of research programme: Ukendt
Amount: 1,263,600.00 Danish Kroner
Source: Unknown
Name of research programme: Ukendt
Amount: 772,800.00 Danish Kroner

**Gas sensitivity of the nanostructured (FeSn)2O3 solid solutions**
The gas-sensitive properties of nanostructured (FeSn)2O3 solid solutions prepared by high-energy ball milling have been investigated in atmospheres containing alcohol, CO, and CH4 gases. It has been found that materials show a high sensitivity with a short response time to the alcohol gas and almost no sensitivity to the other two gases, CO and CH4. Furthermore, it is found that the tin content in alpha-Fe2O3 and tin ions on the surface of alpha-Fe2O3 particles may play
an important role in the enhancement of the gas sensitivity to the alcohol gas.

Department of Physics
Period: 01/01/1997 → ...
Number of participants: 1
Project Manager, organisational:
Jiang, Jianzhong (Intern)

**High-pressure x-ray diffraction**

The use of high pressure as a thermodynamic parameter in the study of solid state phenomena has become increasingly important for basic and applied physics as well as for geophysics. By varying pressure and/or temperature we are able to identify critical thermodynamic coordinates and to monitor how materials transform from one phase to another. In particular, attention is devoted to structural changes, the equation of state, fluctuating valence states, insulator-metal transitions, and the influence of pressure on high Tc superconductors. As for technological applications of high pressure research, one may mention the synthesis of new super hard materials. Our group has pioneered the use of energydispersive methods for high pressure powder x-ray diffraction, in particular in conjunction with synchrotron radiation and the diamond anvil cell. We are also performing high-pressure, high-temperature studies using a large-volume multi-anvil cell. On the technical side, we are developing high-resolution methods based on the image-plate detector.

Department of Physics
University of Copenhagen
Stockholm University
Institute of Low Temperature and Structure Research
Aarhus University
Period: 01/01/1997 → ...
Number of participants: 5
Project participant:
Olsen, J. Staun (Ekstern)
Åbrink, S. (Ekstern)
Waskowska, A. (Ekstern)

**Financing sources**

Source: Unknown
Name of research programme: Ukendt
Amount: 200,000.00 Danish Kroner

**Inter-particle interactions in systems of magnetic nanoparticles**

Magnetic nanoparticles are often found to be superparamagnetic, i.e. the magnetization vector fluctuates among the easy directions of magnetization. We have studied strongly interacting monodisperse particles and have found that the interactions lead to a critical slowing down of the relaxation time and formation of a spin-glass phase below a critical temperature. These phenomena have been studied by Mossbauer spectroscopy and magnetization measurements. Further plans include to determine the critical exponents characterizing the phase transition and to study the dependence of the phase transition temperature on the interaction strength.

Department of Physics
Uppsala University
Period: 01/01/1997 → 31/12/1997
Number of participants: 7
Project participant:
Bødker, Franz (Intern)
Hansen, Mikkel Foug (Intern)
Svedlindh, P. (Ekstern)
Djurberg, C. (Ekstern)
Nordblad, P. (Ekstern)
**Financing sources**
- Source: Unknown
- Name of research programme: Ukendt
- Amount: 853,000.00 Danish Kroner

- Source: Unknown
- Name of research programme: Ukendt
- Amount: 1,065,909.00 Danish Kroner

**M4+ ions in alpha-Fe2O3 structure**
For more than thirty years, it has been assumed that tin ions substitute iron ions in the alpha-Fe2O3 lattice when tin ions dissolve in alpha-Fe2O3 due to the similar ionic size of Fe3+ and Sn4+. No experimental evidence has been reported to examine whether or not the substitution model is valid in this system. We first found that tin ions do not substitute iron ions in the solid solution. The Sn4+ ions occupy the empty octahedral holes in the lattice of the alpha-Fe2O3 phase.

**Proteiners foldning og funktion**
Department of Physics
- Period: 01/01/1997 → 01/08/2002
- Number of participants: 2
- Phd Student: Frimand, Kenneth (Intern)
- Main Supervisor: Bohr, Henrik (Intern)

**Financing sources**
- Source: Internal funding (public)
- Name of research programme: DTU-lønnet stipendie

**Superconducting elements and nonlinearity**

Department of Informatics and Mathematical Modeling
Department of Mathematics
- Period: 01/01/1997 → ...
- Number of participants: 27
- Project participant: Sørensen, Mads Peter (Intern)
- Scott, Alwyn C. (Intern)
- Caputo, Jean Guy (Intern)
- Flytzanis, N. (Ekstern)
- Kalosakas, G. (Ekstern)
- Lazarides, Nikos (Ekstern)
Density Functional Calculations and Molecular Modeling of Biological Ammonia Synthesis

Department of Physics  
Period: 01/12/1996 → 24/03/2000  
Number of participants: 4  
Phd Student:  
Rod, Thomas Holm (Intern)  
Main Supervisor:  
Narskov, Jens Kehlet (Intern)  
Examiner:  
Jacobsen, Karsten Wedel (Intern)  
Stoltze, Per (Intern)

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Grundforskningsfonden-SU  
Project: PhD

Hybrid Electronics of Semiconductors or Semimetals and Superconductors

The project aims at developing the basic know-how for hybrid cryogenic sub-micron scale electronics (nanometer scale electronics). Hybrid combinations of semiconductor-semimetals with superconductor materials are used. Collaboration with Oersted Lab. (NBI) and Danish Institute of Fundamental Metrology.

Department of Physics  
Period: 01/10/1996 → …  
Number of participants: 6  
Project participant:
Elektronstruktur, Binding og Reaktivitet

Department of Physics
Period: 01/09/1996 → 22/09/1999
Number of participants: 4
Phd Student:
Byskov, Line Sjolte (Intern)
Main Supervisor:
Nørskov, Jens Kehlet (Intern)
Examiner:
Chorkendorff, Ib (Intern)
Stoltze, Per (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Grundforskningsfonden-SU
Project: PhD

Projection of computer generated pictures in Tycho Brahe Planetarium, Copenhagen
The aim of the project is to describe the projection of slides with a super wide angel projector on to the dome in the Tycho Brahe Planetarium. A mathematical model of the projection is derived so that computer generated pictures can be “counter destored” prior to projection. First a slide with a well known geometry is projected on to the dome, and the projected picture is measured by means of theodolites. The result is then used to derive the model. In this way correct pictures can be seen by the spectator in the Planetarium.

Department of Applied Civil and Environmental Engineering
Department of Physics
Department of Planning
Operations Research
Department of Informatics and Mathematical Modeling
Tycho Brahe Planetarium
Period: 01/09/1996 → 01/02/1997
Number of participants: 4
Project participant:
Sørensen, Svend Erik Børre (Intern)
Poulsen, Erik Lund (Intern)
Hansen, Per Skafte (Intern)
Project Manager, organisational:
Mærsk-Møller, Ole (Intern)

Biomolekylers fysiske struktur og evolution

Department of Physics
Period: 01/08/1996 → 23/03/2000
Number of participants: 4
Phd Student:
Tøstesen, Eivind (Intern)
Supervisor:
Bohr, Henrik (Intern)
Main Supervisor:
Bohr, Jakob (Intern)
Examiner:
Cotterill, Rodney M J (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-Su Stipendium, Eksperiment
Project: PhD

Ulineære fænomener i biologiske systemer
Department of Physics
Period: 01/08/1996 → 17/05/2000
Number of participants: 2
Phd Student:
Andresen, Peter Ragnar (Intern)
Main Supervisor:
Mosekilde, Erik (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-Su Stipendium, Eksperiment
Project: PhD

Undersøgelser af nye reaktionsveje for ammoniak-synteser på modificerede metal-eenkrystaller
Department of Physics
Period: 01/08/1996 → 16/02/2000
Number of participants: 3
Phd Student:
Dahl, Søren (Intern)
Main Supervisor:
Chorkendorff, Ib (Intern)
Examiner:
Jacobsen, Karsten Wedel (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Grundforskningsfonden
Project: PhD

Undersøgelser af nye reaktionsveje for motand-syntese på modificerede metal-eenkrystaller
Department of Physics
Period: 01/08/1996 → 16/02/2000
Number of participants: 3
Phd Student:
Lorensen, Henrik Qvist (Intern)
Main Supervisor:
Chorkendorff, Ib (Intern)
Examiner:
Schiøtz, Jakob (Intern)

Financing sources
Source: Internal funding (public)
Two-Dimensional Saturation Profiles of Borehole Cores

The principle of the project, which was supported by the EFP-96, was to send a beam of gamma-quanta into the borehole core, and to measure the gamma-quanta which were scattered in the core along the beam by a fixed scattering angle. Through such measurements the saturation profiles may be obtained. Initially a scattering angle of 90° was tried out, but the intensity of the quanta was too low as compared to the background. Later smaller angles were investigated. Unfortunately the project had to be terminated before it was finished because the scientist mainly involved in the project left for a job in industry.

Department of Physics
Period: 01/05/1996 → 31/12/1998
Number of participants: 1
Project Manager, organisational: Ølgaard, Povl Lebeck (Intern)

Phantom models

The project goal has been to establish techniques making it possible to control the perspective effects and stereoscopic parameters in a stereogram independently. Of particular interest is the application of these techniques to obliquely projected stereograms, giving rise to the so-called "Phantom models". The project has led to the submission of a patent application, nr. 00849, priority date 26.06.98. In the interest of prospective license takers, the technical contents of the project are withheld until the expiry of the so-called priority year, i.e. until 26.06.99. The project was supported by Danish Agency for Trade and Industry, total support amounting to D Kr. 180,000. The mediator was Frank Knudsen, Danish technological Institute. Project leader: Svend B. Sørensen, FYS-DTU Project members: Per Skafte Hansen, IMM-DTU Nils Lykke Sørensen, AAA

Department of Physics
Department of Informatics and Mathematical Modeling

Artificial consciousness

This is a formal collaboration with Bjørn Nielsen and Claes Hougaard of Interactive Television Entertainment A/S, and it aims to introduce artificial consciousness to the Internet.

Department of Physics
Interactive Television Entertainment A/S

Chemical Vapour Deposition (CVD)

Der er i samarbejde med NKT Research Center udviklet udstyr for fremstilling af belægninger ved højtemperatur CVD af TiN på metaller samt teknikker for prøvepræparation til TEM-analyse af disse.

Department of Physics

Project: PhD
**Consciousness and Intelligence**
The overall goal of this project is elucidation of the neural correlates of human consciousness and intelligence. An attempt is being made to consolidate anatomical and physiological data into a model that is in agreement with well-established psychophysical facts about consciousness. The work also strives to clarify the nature and determinants of intelligence, from the molecular to the behavioral level.

**Coupled long Josephson junctions**
Fluxon dynamics in long Josephson junctions and interaction between long Josephson junctions are investigated. Two coupling mechanisms have been considered. Magnetic coupling and a direct coupling through the ends of the junctions.

**Determination of two-dimensional saturation profiles in cores by nuclear techniques**

**Examination of physical measurement methods for determination of displacement processes**
In the project is examined the gamma-ray transmission and attenuation method for determination of the flow of oil, gas, and water through chalk reservoirs. Project partners examine other physical methods for obtaining information on the same parameters.
Galvaniske belægninger
I samarbejde med Forskningscenter Risø og Center for Avanceret Galvanoteknik er mikrostrukturer og styrke af
Elektrokemisk udfældet nikkel og krom samt kobber/nikkel multilag blevet undersøgt.

Department of Physics
Risø National Laboratory for Sustainable Energy
Center for Avanceret Galvanoteknik
Period: 01/01/1996 → ...
Number of participants: 3
Project participant:
Nielsen, Christian Bergenstof (Intern)
Bohr, Jakob (Intern)

Intrinsic and stacked Josephson junctions
Research has been carried out in order to clarify the complicated dynamics taking place in intrinsic Josephson junctions of
the type BSCCO. Model equations has been set up and numerical simulations performed. Experiments on low Tc model
systems as well as single crystal BSCCO samples has been performed. An invited lecture at the M2SHTSC conference in
Beijing summarised some of the main results obtained.

Department of Physics
Period: 01/01/1996 → 31/12/1996
Number of participants: 5
Project participant:
Sakai, Shigeki (Ekstern)
Muller, Paul (Ekstern)
Ustinov, Alexey (Ekstern)
Cirillo, Matteo (Ekstern)

Molecular Genetics of Autism.
This formal collaboration aims at finding all the genes implicated in autism. It involves tests on blood samples taken from
multiplex families (i.e. families in which there is more than one affected child). The partners include Sir Michael Rutter and
Anthony Bailey, Institute of Psychiatry, London; Anthony Monaco at the Wellcome Institute of Human Genetics, Oxford;
and many other collaborators in England (Anne Le Couteur et al.), USA (Cathy Lord et al.), Germany (Fritz Poustka et al.),
Holland (Herman van Engeland, Chantal Kemner et al.), France. The other Danish members of the Consortium are Karen
Brøndum-Nielsen, J F Kennedy Institute, Glostrup; Demetrious Haracopoulos and Lennart Pedersen, Videncenter for Autism,
Virum; and Torben Isager, Glostrup Amtssygehus.

Department of Physics
Period: 01/01/1996 → …
Number of participants: 1
Project Manager, organisational:
Cotterill, Rodney M J (Intern)

Project

Nonlinear properties of long Josephson junctions
Soliton dynamics of long Josephson junctions has been investigated. The role of geometrical and temperature gradients
has been investigated in detail. The analytical results has been compared with experiments on superconducting structures
with different geometries

Department of Physics
Period: 01/01/1996 → 31/12/1996
Number of participants: 1
Project Manager, organisational:
Pedersen, Niels Falsig (Intern)

Project

Surface properties and magnetic relaxation of metallic iron nanoparticles
We have studied nanoparticles of metallic iron with sizes of 2-4 nm which are very difficult to handle as they will oxidize
immediately in the presence of oxygen. Therefore we have developed a new type of in situ cell which allows us to perform
Mössbauer spectroscopy under optimal condition with the possibility of controlling the environment of the particles. With
this type of cell we were also able to perform magnetization measurements and neutron scattering. Nanoparticles have a
large fraction of their atoms in the surface and the particles will therefore be influenced by the properties of the surface
atoms. Such small particles are thus very sensitive to chemisorption of gasses. With Mössbauer spectroscopy we have
studied the effect of chemisorption of oxygen, carbon monoxide and nitrogen on the surface. We found that oxygen results
in a ferromagnetic oxide overlayer, while carbon monoxide results in diamagnetism and nitrogen gives a broad distribution
of magnetic moment in the particle surface. Due to the small size of the nanoparticles it is possible to observe size effects
such as superparamagnetic relaxation which is a thermally activated fluctuation of the magnetic particle moment. The
frequency of these fluctuations was found to vary 11 orders of magnitude in the studied temperature range in good
agreement with theoretical predictions. These results are among some of the first consistent measurements of this type
and the very first on metallic iron particles.

Department of Physics

Hempel A/S
Uppsala University
Centro Politecnico Superior de Ingenieros
Period: 01/01/1996 → 31/12/1996
Number of participants: 9
Project participant:
Mørup, Steen (Intern)
Rasmussen, Helge Kildahl (Intern)
Chorkendorff, Ib (Intern)
Pedersen, Michael S. (Ekstern)
Svedlindh, Peter (Ekstern)
Jonsson, G. T. (Ekstern)
Garcia-Palacios, J.L. (Ekstern)
Lazaro, F.J. (Ekstern)
Project Manager, organisational:
Bødker, Franz (Intern)

Financing sources
Source: Unknown
Name of research programme: Ukendt
Amount: 832,000.00 Danish Kroner
**Væske-faststof interfaces**
Væske-faststof-interfaces undersøges ved atomic force og scanning tunneling mikroskopi med henblik på bestemmelse af interface-spændinger i væsken og lokalisering af heraf frembragte kavitationskerner (hulrum) i forhold til den faste overflades topografi.

Department of Physics  
Period: 01/01/1996 → …  
Number of participants: 1  
Project Manager, organisational:  
March, Knud Aage (Intern)

**Magnetiske nanopartikler**

Department of Physics  
Period: 01/10/1995 → 11/02/1999  
Number of participants: 2  
Phd Student:  
Hansen, Mikkel Fougt (Intern)  
Main Supervisor:  
Mørup, Steen (Intern)

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Forskningsrådsstip.-SU, Eksp  
Project: PhD

**Reactivity of Pure and Modified Surfaces - a Supersonic Molecular Beam Approach**

Department of Physics  
Period: 01/10/1995 → 14/12/1998  
Number of participants: 4  
Phd Student:  
Nielsen, Jane Hvobæk (Intern)  
Main Supervisor:  
Chorkendorff, Ib (Intern)  
Examiner:  
Luntz, Alan (Ekstern)  
Stoltze, Per (Intern)

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: DTU-Su Stipendium, Eksperiment  
Project: PhD

**Fremstilling af YBa2Cu3O7-x Højtemperatur**

Department of Physics  
Period: 01/09/1995 → 31/12/1996  
Number of participants: 3  
Phd Student:  
Tidemand-Petersson, Camilla (Intern)  
Supervisor:  
Høj, Jakob Weiland (Intern)  
Main Supervisor:  
Mygind, Jesper (Intern)

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Anden Offentlig Finansier-SU
Project: PhD

Risks Associated with Old Nuclear Submarines in Russia
In an international NATO/NACC project under the Committee of the Challenges of Modern Society the risks of the old, decommissioned nuclear submarines at the Kola peninsula have been investigated. The Danish contribution to this project was an analysis of the potential sources of radioactive pollution from these submarines, the development of a model for calculation the energy release connected to a criticality accident during defueling and an analysis of available information on accidents with nuclear submarines.

Department of Physics
Period: 01/09/1995 → 31/12/1998
Number of participants: 1
Project Manager, organisational: Ølgaard, Povl Lebeck (Intern)

Structural studies of inorganic materials
Crystal structures, i.e. the atomic arrangements in crystalline materials, form the basis for our understanding and development of inorganic materials. In this project crystal structures are determined and studied by means of single-crystal and powder diffraction methods using conventional and synchrotron X-rays, as well as neutron sources. It is also the aim of this project to explore the possibilities and develop crystallography as a tool for structural studies. The crystallographic studies are complemented by electron microscopy, spectroscopy, thermal, electro-chemical and kinetic methods. Among the materials studied are vanadium containing catalysts, where the catalytic properties are relying on the variability of the oxidation state of vanadium, which in turn depends on the structure hosting the vanadium ions. Another group of materials studied is optically and electro-optically active ceramics, whose polar properties can be directly related to their atomic arrangements. In yet another group of materials, minerals, new structures are determined and structurally related to known materials, and the stability fields and structural variations of solid solutions are explored.

Department of Chemistry
Indoor Environment
Department of Mechanical Engineering
Department of Physics
University of Milan
Lund University
Chalmers University of Technology
University of Copenhagen
Brookhaven National Laboratory

Period: 01/09/1995 → …
Number of participants: 10
Project participant:
Nielsen, Kurt (Intern)
Artioli, Gilberto (Ekstern)
Hansen, Staffan (Ekstern)
Albertsson, Jørgen (Ekstern)
Johnsen, Ole (Ekstern)
Hansen, Jonathan (Ekstern)
Fehrmann, Rasmus (Intern)
Eriksen, Kim Michael (Intern)
Jiang, Jianzhong (Intern)
Project Manager, organisational: Ståhl, Kenny (Intern)

Financing sources
Source: Unknown
Name of research programme: Ukendt
Amount: 15,000.00 Danish Kroner
Project
Ceramic Conductors and Superconductors: Materials and Devices
The aim of this project is to maintain a state-of-the-art deposition facility for high quality yttrium-barium-copper-oxide (YBCO) superconducting films and to characterize ceramic thin-films as well as prototype thin-film devices such as Josephson junctions and SQUIDs. Thin-films are fabricated using a pulsed laser deposition set-up with a Questek 2720 excimer laser, scanning optics, and a chamber which allows deposition in a controlled low-pressure oxygen/argon atmosphere. Basic equipment for lithography (wet etching) is available. A range of characterization equipment for determining e.g. electric and magnetic properties down to low temperatures is employed in the studies. In 1999 the activities have been: 1) studies of flux noise in ceramic high-critical temperature (high Tc) superconducting thin films, Josephson junctions and SQUIDs (two M.Sc. projects with NKT Research Center) and 2) application of high-Tc SQUIDs to studies of magnetic fields generated by peripheral nerve currents (ph.d. projects with NKT Research Center and the Copenhagen University Teaching Hospital Rigshospitalet).

Department of Physics
Risø National Laboratory for Sustainable Energy
NKT Research & Innovation A/S
Period: 01/07/1995 → …
Number of participants: 6
Project participant:
Hansen, Jørn Bindslev (Ekstern)
Skov, Johannes (Intern)
Rasmussen, Inge (Intern)
Linderoth, Søren (Intern)
Shen, Y. (Ekstern)
Project Manager, organisational:
Jacobsen, Claus Schelde (Intern)

Financing sources
Source: Unknown
Name of research programme: Ukendt
Amount: 180,000.00 Danish Kroner

Integrated High Critical Temperature Superconducting Components
The aim of this project is to investigate the potential of Rapid Single Flux Quantum (RSFQ) elements for high frequency electronics and the properties of the devices. Using flux quantization in Superconducting QUantum Interference Devices (SQUIDs) the magnetic flux quanta can be used as the units of digital information. Combining SQUIDs in an appropriate manner one can built digital logical circuits. The goal is to investigate the properties of some logical circuits made of high-Tc superconductors.

Department of Physics
NKT Research Center Ltd.
Period: 01/07/1995 → 31/12/1998
Number of participants: 4
Project participant:
Mygind, Jesper (Intern)
Pedersen, Niels Falsig (Intern)
Jacobsen, Claus Schelde (Intern)
Project Manager, organisational:
Fischer, Gerd Michael (Intern)

Financing sources
Source: Unknown
Name of research programme: Ukendt
Amount: 600,000.00 Danish Kroner

Nonlinear Dynamics of a Vectored Thrust Aircraft
Thrust vectoring allows an aircraft to venture into regions of operation that cannot be reached with conventional controls. Using data for the aerodynamic coefficients obtained by NASA, we have performed a detailed simulation study of the longitudinal dynamics of the F/A-18 fighter in the poststall regime. Under variation of the thrust and the thrust vectoring...
angle, the equilibrium state exhibits three Hopf bifurcations and two saddle-node bifurcations. The purpose of the project is to examine the additional bifurcations that arise under sinusoidal forcing of the thrust vectoring angle.

Department of Physics
Budapest University of Technology and Economics
Period: 01/07/1995 → 31/12/1998
Number of participants: 2
Project participant:
Granasy, Peter (Ekstern)
Project Manager, organisational:
Mosekilde, Erik (Intern)

Investigation of borehole cores with four different, physical methods
The project which was supported by EFP-95, investigated the saturation profiles of borehole cores by use of four different methods, gamma-transmission, electric impedance, NMR and CT-scanning. Four institutes, three at TUD and one at GEUS, each examined one method. The gamma-transmission method was considered in a cooperation between the Institute of Physics and the Institute of Automation. An experimental facility was built by use of which measurements on borehole cores with various water, oil and gas saturations were performed. In addition a computer programme that calculated the saturations from the measurements was prepared. The results obtained look promising, but the preparation of the cores involved so large an effort that only three borehole cores could be measured. This is enough to pass final judgement on the method.

Department of Physics
Period: 01/05/1995 → 31/12/1998
Number of participants: 1
Project Manager, organisational:
Ølgaard, Povl Lebeck (Intern)

Quantum phenomena in mesoscopic superconductor semiconductor devices
The project aims at developing a new type of fast three terminal electronic devices based on superconductor/semiconductor (S/Sm) interfaces, and to gain a better fundamental understanding of the quantum mechanical processes responsible for the so-called proximity effect between normal conductors and superconductors. The hybrid S/Sm devices composed of Aluminium (S) and Gallium Arsenide (Sm), developed and used in the project, are synthesized by thin film crystal growth techniques in a molecular beam epitaxy (MBE) ultra high vacuum chamber, and subsequently processed by photo- and electron beam lithography. The MBE technique allows a control of the crystal growth on atomic monolayer scale, while electron beam lithography is used to achieve sub micrometer lateral spacing between adjacent superconducting contacts to the semiconductor. In order to reach below the critical temperature of Aluminium (1.2 K) the electronic transport in the devices is studied at cryogenic temperatures down to 300 mK.

Department of Physics
University of Copenhagen
Period: 01/03/1995 → …
Number of participants: 8
Project participant:
Hansen, Jørn Bindslev (Ekstern)
Jacobson, Claus Schelde (Intern)
Skov, Johannes (Intern)
Rasmussen, Inge (Intern)
Kutchinsky, Jonatan (Intern)
Lindelof, Poul Erik (Ekstern)
Serensen, Claus B. (Ekstern)

Project Manager, organisational:
Taboryski, Rafael J. (Intern)

Financing sources
Source: Unknown
Name of research programme: Ukendt
Amount: 1,107,557.00 Danish Kroner
**Dissociation af N₂ på Fe (III)**

Department of Physics  
Period: 01/02/1995 → 28/04/1998  
Number of participants: 4  
Phd Student:  
Mortensen, Jens Jørgen (Intern)  
Supervisor:  
Jacobsen, Karsten Wedel (Intern)  
Main Supervisor:  
Nørskov, Jens Kehlet (Intern)  
Examiner:  
Chorkendorff, Ib (Intern)

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: DTU-Su Stipendium, Eksperiment  
Project: PhD

**Fasekonjugerede lasere**

Department of Physics  
Period: 01/02/1995 → 28/08/1998  
Number of participants: 4  
Phd Student:  
Løbel, Martin Bo Hjort (Intern)  
Supervisor:  
Johansen, Per Michael (Intern)  
Main Supervisor:  
Buchhave, Preben (Intern)  
Examiner:  
Skettrup, Torben (Intern)

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Forskerakademiets Samfinansier  
Project: PhD

**Cryogenic scanning micro and nanoprobes (CSLM, STM)**

A Cryogenic Scanning Laser Microscope (CSLM) is being developed. The sample placed on a chip is locally heated by laser power from a glass fibre, that is x-y scanned across the sample within a distance of a few microns. The spatial resolution is approx. 2 micrometer, given by the thermal healing length. The sample response is used to study the properties of the device under test. A miniature Scanning Tunneling Microscope (STM) with atomic resolution is under construction. It can be operated at millikelvin temperatures and will be used for the study of noise and dynamics of nanostructures.

Department of Physics  
Department of Hydrodynamics and Water Resources  
Danish Institute of Fundamental Metrology  
Lucent Technologies Denmark A/S  
Teleteknisk Forskningslaboratorium  
Period: 01/01/1995 → …  
Number of participants: 2  
Project participant:  
Holm, Jesper (Intern)  
Project Manager, organisational:  
Mygind, Jesper (Intern)

**Financing sources**
Den avancerede kongendevandsreaktor med naturlig cirkulation

Department of Physics
Number of participants: 4
PhD Student:
Metz, Hans Peter (Intern)
Main Supervisor:
Ølgaard, Povl Lebeck (Intern)
Examiner:
Johansson, Torben (Intern)
Thorlaksen, Bjørn (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Risø (Løn)
Project: PhD

Dislokationens struktur og dynamik

Department of Physics
Period: 01/01/1995 → 25/02/1998
Number of participants: 3
PhD Student:
Rasmussen, Torben (Intern)
Main Supervisor:
Jacobsen, Karsten Wedel (Intern)
Examiner:
Skriver, Hans Lomholt (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Risø (Løn)
Project: PhD

Electronic devices based on Single Electron Tunneling (SET)
Future electronics is expected to be based on quantum mechanical tunneling of single electrons and/or Cooper pairs (SET and/or CPT) in extremely small structures (mesoscopic or nanostructures). The simplest three-terminal device is the SET transistor. The project includes experimental and theoretical studies of the noise and nonlinear properties of SET devices. The experiments require very careful electrical shielding and millikelvin temperatures. In metrology the SET devices have future applications as current standards and extremely sensitive electrometers.

Department of Physics
Danish Institute of Fundamental Metrology
Moscow State University
National Institute of Standards and Technology
Physikalisch-Technische Bundesanstalt
Period: 01/01/1995 → …
Number of participants: 5
Project participant:
Samuelsen, Mogens Rugholm (Intern)
Manscher, Martin (Intern)
Qualmøn, Werner (Intern)
Ejrnæs, Mikkel (Intern)
Project Manager, organisational: 
Mygind, Jesper (Intern)

Financing sources
Source: Unknown
Name of research programme: Ukendt
Amount: 100,000.00 Danish Kroner
Source: Unknown
Name of research programme: Ukendt
Amount: 40,000.00 Danish Kroner
Source: Unknown
Name of research programme: Ukendt
Amount: 750,000.00 Danish Kroner

Forudsigelse af oprindelig form ud fra kendskab til massefordeling af fragmenter - anvendelse i arkeologien

Department of Physics
Period: 01/01/1995 → …
Number of participants: 2
Project participant:
Oddershede, Lene (Intern)
Project Manager, organisational:
Bohr, Jakob (Intern)

Fundamentale virkemåder af tapping mode atomic force mikroskop
Ved "tapping mode" AFM vibreres mikroskopets bladfjeder, hvorpå selve proben befinder sig, ved fjederens resonansfrequens. Dette gøres i en sådan højde fra prøven, at proben periodisk er i kontakt med prøven - den "tapper". Denne mode er særdeles velegnet til mikroskopering af bl.a. løse partikler på overflader, da de laterale kræfter i denne mode er små. Metoden er relativ ny, og der er derfor mange uafklarede spørgsmål, f.eks. omkring størrelsen af de involverede kræfter, samt om hvordan man bør indstille mikroskopet (amplitude, frekvens etc.) for at udnytte metoden optimalt. Vi har eksperimentelt gjort vigtige opdagelser desangående og arbejder med at undersøge disse ved yderligere målinger samt ved numeriske simuleringer.

Department of Physics
Department of Electric Power Engineering
Period: 01/01/1995 → …
Number of participants: 4
Project participant:
Sørensen, Alexis Hammer (Intern)
Mørch, Knud Aage (Intern)
Kyhle, Anders (Intern)
Project Manager, organisational:
Bohr, Jakob (Intern)

Indikationer om meteoriters form fra scaling eksponenter i massefordelinger fra meteorit showers
Massefordelingerne af fragmenter fra meteorit showers udviser scaling over flere dekader, og de observerede scaling eksponenter varierer fra shower til shower. Scaling analysen giver information om fragmentations processen og om egenskaber af den meteoroid, som blev fragmenteret ved sammenstødet med jordens atmosfære. De observerede scaling eksponenter kan sammenlignes med eksponenter fundet i laboratorieforsøg, hvor man iagttagt, at eksponenterne afhænger af den oprindelige form. Således åbnes mulighed for, at man kan udlede information om meteroidens oprindelige form.
Molekylær biofysik
Der arbejdes på at opnå en dybere forståelse af strukturdannelsen i biomolekylære kædemolekyler, som f.eks. proteiner og DNA.

Molekylær bioinformatik
Der arbejdes på at klassificere de statistiske afstandsforhold i proteiner i minimale sæt. Efterfølgende anvendes disse sæt til forudsigelser af proteinstruktur og egenskaber.

Oscillators based on dynamics of magnetic flux quanta (FFO)
Flux Flow Oscillators (FFO) are tuneable in the frequency range 200-600 GHz by the applied dc bias current and magnetic field. FFOs are potential local oscillators for SiS mixers in integrated fully superconducting submillimeter astronomical and space borne receivers with low noise and fine spectral resolution. The project is mainly concerned with experimental and theoretical investigations of the fluxon dynamics and noise mechanisms behind the dc properties and the intrinsic spectral width of the emitted radiation. A linewidth as low as 140 kHz has been measured at 450 GHz. Frequency and phase locking of the FFO is planned.
Scanning probe mikroskopi (AFM/STM) af nanopartikler deponeret på flade substrater

Ønsket om hurtigere og mere kompakt elektronik krav til halvlederindustrien om udvikling af elektroniske kredsloeb på nanometer skala (10-100 nm). Komponenter i denne størrelse vil endvidere give mulighed for at udnytte kvante-effekter ved stuetemperatur. Med nuværende litografiske tekniker er det meget kompliceret at fabrikere sådanne komponenter (strukturen), og vejen til produktion i stor skala synes lang, dersom man kunne benytte nanopartikler (der er relativt lette at fremstille) til disse kredsloeb. Særligt om man kunne bringe nanopartiklerne til at selv-organisere i regulære strukturer (arrays). Nærværende projekt består af AFM/STM mirkoskopering af overflader dækket med nanopartikler (klynger) for at studere forholdene omkring organiseringen af partiklerne. Der er observeret meget interessante fænomener som f.eks. ”perlekæder” af partikler, der er dannet spontant i forbindelse med deponeringen af partiklerne. Prøverne bliver hovedsageligt fabrikeret af vore samarbejdspartnere i Klyngegruppen på Niels Bohr Institutet, men gruppen fremstiller også selv prøver ud fra kemisk fremstillede nanopartikler. Endvidere er en opstilling til vakuum deponering af nanopartikler under indkøring (fagpakkeprojekt). Arbejdet foregår inden for rammerne af MUP2 centersamarbejdet CNAST.

Department of Physics
Department of Electric Power Engineering
Niels Bohr Institute
Period: 01/01/1995 → …
Number of participants: 4
Project participant:
Sørensen, Alexis Hammer (Intern)
Mørch, Knud Aage (Intern)
Kyhle, Anders (Intern)
Project Manager, organisational:
Bohr, Jakob (Intern)

Selv-organiserede makroskopiske strukturer i magnetiske væsker

Når en dråbe magnetisk væske omgivet af vand i en Hele-Shaw celle påtrykkes et ydre magnetisk felt vinkelret på cellens overflade, vil dipol-dipol vekselvirkningen i den magnetiske væske i konkurrence med overfladespænding mellem vang og ferrofluiden bevirke, at der dannes fantastiske mønstre: labyrintiske, dråbeagtige, eller kaotiske. Disse mønstre er yders følsomme over for randværdi og begyndelsesbetingelser i forsøget såsom magnetfeltets størrelse tidslige udviklingen, cellens højde og brøkdelen af ferrofluid i cellen. Der arbejdes på at beskrive og få en forenet forståelse af alle disse fænomener.

Department of Physics
Period: 01/01/1995 → …
Number of participants: 2
Project participant:
Oddershede, Lene (Intern)
Project Manager, organisational:
Bohr, Jakob (Intern)

Stereoskopi 1 : ColorCode 1995 - 2003


Department of Informatics and Mathematical Modeling
Department of Physics
Technical University of Denmark
Period: 01/01/1995 → 31/12/2003
Number of participants: 1
Project Manager, organisational:
Hansen, Per Skafte (Intern)
**AFM/STM studier af klynger og større molekyler samt disseks selvorganisering på overflader**

Department of Physics  
Period: 01/12/1994 → 25/02/1998  
Number of participants: 3  
Phd Student:  
Sørensen, Alexis Hammer (Intern)  
Supervisor:  
Mørch, Knud Aage (Intern)  
Main Supervisor:  
Bohr, Jakob (Intern)

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Program Stipendium-SU, Eksp  
Project: PhD

**Nanostructures for X-ray optics**

The project, performed by Salim Abdali, aims at studying multilayers and other X-ray optical elements with potential use in X-ray astronomy in the photon energy ranges below 0.2 keV and around the Fe K alpha line at 6.9 keV. The project is a collaboration with Finn E. Christensen of the Danish Space Research Institute. Multilayers of Co/C have been deposited on Si 111 crystals for simultaneous spectroscopy of soft and hard X-rays, utilizing diffraction in the multilayers and the substrate, respectively. In addition, LiF 220 and RAP crystals are included in the Bragg reflection panel of the Russian-Danish satellite SRG, provided with a Wolther Type I telescope. The latter has been tested at the synchrotron radiation source of the Daresbury Laboratory in England.

Department of Physics  
Niels Bohr Institute  
Stockholm University  
Institute of Low Temperature and Structure Research  
Period: 01/11/1994 → 31/12/2000  
Number of participants: 6  
Project participant:  
Jiang, Jianzhong (Intern)  
Mørup, Steen (Intern)  
Staun Olsen, J. (Ekstern)  
Åsbrink, S. (Ekstern)  
Waskowska, A. (Ekstern)  
Project Manager, organisational:  
Gerward, Leif (Intern)

**Financing sources**  
Source: Unknown  
Name of research programme: Ukendt  
Amount: 200,000.00 Danish Kroner  
Project

**Nanostrukturer til røntgenoptik**

Department of Physics  
Number of participants: 3  
Phd Student:  
Abdali, Salim (Intern)  
Main Supervisor:  
Gerward, Leif (Intern)  
 Examiner:  
Mørch, Knud Aage (Intern)
Financing sources
Source: Internal funding (public)
Name of research programme: Anden Offentlig Finansier-SU
Project: PhD

Tribologi på Atomart Niveau
Department of Physics
Period: 01/09/1994 → 23/10/1997
Number of participants: 4
Phd Student: Sørensen, Mads Reinholdt (Intern)
Supervisor: Nørskov, Jens Kehlet (Intern)
Main Supervisor: Jacobsen, Karsten Wedel (Intern)
Examiner: Bøttiger, Jørgen (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-Su Stipendium, Eksperiment
Project: PhD

Forcerde og koblede ikke-lineære oscillatorer
Department of Physics
Period: 01/08/1994 → 01/10/1997
Number of participants: 3
Phd Student: Olesen, Michael Wiinberg (Intern)
Supervisor: Knudsen, Carsten (Intern)
Main Supervisor: Mosekilde, Erik (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-Su Stipendium, Eksperiment
Project: PhD

Optical non-linear wave guides with quasi phase matching
Non-linear optical effects in wave guides are investigated in LiNbO3. Wave guides suited for frequency doubling are designed and constructed. Phase matching by means of periodically poled ferroelectric domains is investigated.

Department of Physics
Period: 01/07/1994 → 01/05/1996
Number of participants: 1
Project Manager, organisational: Skettrup, Torben (Intern)

Teori for STM
Department of Physics
Period: 01/03/1994 → 26/08/1997
Number of participants: 3
Phd Student: Brandbyge, Mads (Intern)
Main Supervisor: Jacobsen, Karsten Wedel (Intern)
Examiner:
Svane, Axel (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Grundforskningsfonden-SU
Project: PhD

Tyndfilmlysbeigeledere
Department of Physics
Period: 01/02/1994 → 30/04/1997
Number of participants: 4
Phd Student:
Veng, Torben Erik (Intern)
Main Supervisor:
Sktetrup, Torben (Intern)
Examiner:
Bozhevolnyi, Sergey I. (Intern)
Leistiko, Otto (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-Su Stipendium, Eksperiment
Project: PhD

Diodelaser pumpede faststoflaser systemer
Department of Physics
Period: 01/12/1993 → 03/06/1997
Number of participants: 2
Phd Student:
Tidemand-Lichtenberg, Peter (Intern)
Main Supervisor:
Buchhave, Preben (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsstip.-SU, Eksp
Project: PhD

Alloys, multilayers, and interfaces
The goal of the project is to be able to design alloy systems with desirable physical and chemical properties. We also aim at developing theories of alloy formation, heats of solution, and segregation including structural effects. This is achieved through total energy calculations performed within density functional theory. The project involves studies of random as well as partially and completely ordered alloy systems in configurations including multilayers, interfaces, and surfaces. We also study surface alloys. Part of the project involve the development of more accurate but still efficient computational procedures for bulk, surface, and interface systems.

Department of Physics
MPI

Janos Kollár
Uppsala University
Period: 01/09/1993 → …
Number of participants: 5
Project participant:
Ruban, Andrei (Intern)
Andersen, O.K. (Ekstern)
Johansson, Börje (Ekstern)
Vitos, Levente (Ekstern)
Project Manager, organisational:
Skriver, Hans Lomholt (Intern)

Financing sources
Source: Unknown
Name of research programme: Ukendt
Amount: 1,000,000.00 Danish Kroner

Electronic structure and reactivity
The project aims at developing models of adsorption and reaction at surfaces. The basis is detailed self-consistent calculations using density functional theory with a non-local desorption of exchange and correlation. Models based on the effective medium theory and the Newns-Andersen model are developed to identify the important parameters determining the reactivity of a given system. The theoretical work is closely coupled to experiments on model systems and in industry. The systems studied include clean metals, alloys, transition metal sulfides, and models of enzymes.

Department of Physics
Aarhus University
Haldor Topsoe AS
Veronica Pirovano
Period: 01/09/1993 → ...
Number of participants: 13
Project participant:
Jacobsen, Karsten Wedel (Intern)
Stoltze, Per (Intern)
Byskov, Line Sjolte (Intern)
Rod, Thomas Holm (Intern)
Mavrikakis, Manos (Intern)
Bengaard, Hanne Skov (Intern)
Logadottir, Ashildur (Intern)
Bollinger, Mikkel (Intern)
Besenbacher, Flemming (Ekstern)
Stensgaard, Ivan (Ekstern)
Laegsgaard, Erik (Ekstern)
Clausen, Bjørne S. (Ekstern)
Project Manager, organisational:
Nørskov, Jens Kehlet (Intern)

Financing sources
Source: Unknown
Name of research programme: Ukendt
Amount: 1,000,000.00 Danish Kroner
Source: Unknown
Name of research programme: Ukendt
Amount: 290,000.00 Danish Kroner
Source: Unknown
Name of research programme: Ukendt
Amount: 145,000.00 Danish Kroner
Source: Unknown
Name of research programme: Ukendt
Amount: 224,000.00 Danish Kroner

Interatomare vekselvirkninger i metaller.
Department of Physics
Period: 01/09/1993 → 27/01/1997
Number of participants: 3
Phd Student:
Christensen, Asbjørn (Intern)
Metallic nanostructures
The aim of the project is to study the mechanisms behind the formation of metallic nanostructures and to investigate the structural, mechanical, and electrical properties of nanostructures. The project has involved studies of atomic mobility at surfaces and the aggregation of adatoms into islands of various morphologies. Also investigations of mechanical and electrical aspects of a scanning-tunneling-microscope tip interacting with a metal surface have been carried out. In particular the tip-surface system has been used as a model system for nanotribological considerations. Finally, a series of simulations of plastic deformation of nanophase metals have been performed.

Department of Physics
Aarhus University
Period: 01/09/1993 → …
Number of participants: 12
Project participant:
Stoltze, Per (Intern)
Nørskov, Jens Kehlet (Intern)
Schiøtz, Jakob (Intern)
Nielsen, Ole Holm (Intern)
Vegge, Tejs (Intern)
Bahn, Sune Rastad (Intern)
Lorensen, Henrik Qvist (Intern)
Bollinger, Mikkel (Intern)
Besenbacher, Flemming (Ekstern)
Stensgaard, Ivan (Ekstern)
Lægsgaard, Erik (Ekstern)
Project Manager, organisational:
Jacobsen, Karsten Wedel (Intern)

Financing sources
Source: Unknown
Name of research programme: Ukendt
Amount: 1,000,000.00 Danish Kroner
Source: Unknown
Name of research programme: Ukendt
Amount: 172,000.00 Danish Kroner
Source: Unknown
Name of research programme: Ukendt
Amount: 103,000.00 Danish Kroner

Simulations of alloy dynamics and kinetics
In this project the macroscopic properties of systems are determined based on description at the atomic level through large-scale computer simulations. The main topics of interest are the stability, structure and dynamics of alloys and of metal surfaces and the relation between observed kinetics and reaction mechanism for industrial catalytic reactions. Some of the software for simulation and visualization is available at http://www.fysik.dtu.dk/camp-sd.html

Department of Physics
Haldor Topsoe AS
Period: 01/09/1993 → …
Number of participants: 10
Project participant:
Studier af simple molekylers klæbningskoefficient og dynamik på metal-enkystaloverflader ved hjælp af supersoniske molekystråler.

Department of Physics
Period: 01/09/1993 → 07/06/1996
Number of participants: 4
Phd Student: Holmblad, Peter Mikal (Intern)
Main Supervisor: Chorkendorff, Ib (Intern)
Examiner: Alstrup, Ib Andersen (Ekstern)
Jacobsen, Karsten Wedel (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Anden Forskningsrådsfinan.-SU
Project: PhD

Surface reactivity
Fundamental research of surface reactivity is imperative for understanding technological important processes such as catalysis, corrosion, adhesion, etc., where bonds are created or breaking at the surface. By studying the gas-surface interaction under well defined conditions, the elementary steps, in for example a catalytical process, can be investigated in detail on the molecular level. Most of the efforts are focused on understanding the fundamental behavior of this reactivity as a function of the surface composition and structure. By combining Ultra High Vacuum equipment and high pressure cells or supersonic molecular beams the surface reactivity of metal overlayers or surface alloys prepared in situ can be measured. The surfaces are characterized by using a complementary range of surface sensitive methods such as XPS, AES, SAM, LEED, HREELS, TPD, and STM. The results form a basis for revealing the underlying principles of surface reactivity and thereby serve as an inspiration source for designing new catalysts or schemes for preventing surface corrosion. The processes studied are of relevance for some major large scale chemical processes, such as methanol synthesis, ammonia synthesis, steam reforming, and metal dusting, the latter being a corrosion phenomena.

Department of Physics
Haldor Topsoe AS
Period: 01/09/1993 → …
Number of participants: 8
Project participant:
Dahl, Søren (Intern)
Larsen, John (Intern)
Sckerl, Susanne Quist (Intern)
Egeberg, Rasmus (Intern)
Waltenburg, Hanne Neergaard (Intern)
Turing Structures in the CIMA Reaction
The two-species reaction-diffusion model developed by Lengyel and Epstein represents a key to understanding the recently observed Turing structures in the chlorite-iodide-malonic acid (or CIMA) reaction. In this project we study the emergence, growth, competition and final stabilization of various concentration patterns through numerical simulation of the CIMA model. Special emphasis is given to studying the stable localized structures rendered possible by the strongly subcritical character of the Turing bifurcation.
Supervisor:
Johansen, Per Michael (Intern)
Main Supervisor:
Buchhave, Preben (Intern)
Examiner:
Skettrup, Torben (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskerakademiets Samfinansier
Project: PhD

Superferromagnetske Nanostrukture.
Department of Physics
Period: 01/02/1993 → 09/05/1996
Number of participants: 2
Phd Student:
Pedersen, Michael Stanley (Intern)
Main Supervisor:
Mørup, Steen (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsstip.-SU, Eksp
Project: PhD

Inorganic Catalysis
Multidisciplinary investigations of structure and catalytic activity of inorganic catalysts and model systems. In collaboration with ICAT.
Department of Chemistry
Department of Physics
Department of Chemical and Biochemical Engineering
University of Patras
Université de Provence
Institute of Catalysis
Georgia Institute of Technology
B.P. Chemicals SA
Haldor Topsoe AS
University of Copenhagen
Period: 01/01/1993 → ...
Number of participants: 25
Project participant:
Eriksen, Kim Michael (Intern)
Berg, Rolf W. (Intern)
Holten, Bodil Filis (Intern)
Nielsen, Kurt (Intern)
Rasmussen, Søren Birk (Intern)
Mattsson, Rikke Christina (Intern)
Barfod, Rasmus (Intern)
Riisager, Anders (Intern)
Boghosian, Soghomon (Ekstern)
Hatem, Gerard (Ekstern)
Gaune-Escard, Marcelle (Ekstern)
Balzhinimaev, Bair (Ekstern)
Lapina, Olga (Ekstern)
Winnick, Jack (Ekstern)
Oehlers, Cord (Ekstern)
Schoubye, Peter (Ekstern)
Topsøe, Nan Yu (Ekstern)
Hyldtoft, Jens (Ekstern)
Thorhauge, Max (Ekstern)
Gabrielsson, Per (Ekstern)
Teunissen, Herman (Ekstern)
Møller, Preben Juul (Ekstern)
Chorkendorff, Ib (Intern)
Hjortkjær, Jes (Intern)
Project Manager, organisational:
Fehrmann, Rasmus (Intern)

Financing sources
Source: Unknown
Name of research programme: Ukendt
Amount: 345,000.00 Danish Kroner
Source: Unknown
Name of research programme: Ukendt
Amount: 28,000.00 Danish Kroner
Source: Unknown
Name of research programme: Ukendt
Amount: 6,100,000.00 Danish Kroner
Source: Unknown
Name of research programme: Ukendt
Amount: 185,000.00 Danish Kroner

Numerical and Experimental Fluid Mechanics
STVF Framework Programme Subtask: Development of Particle Image Velocimetry (PIV) for the study of turbulence modelling. Subtask: Measurements in turbulent flows
Department of Physics
Period: 01/01/1993 → …
Number of participants: 1
Project Manager, organisational:
Buchhave, Preben (Intern)

Ulinære egenskaber af optiske tyndfilm.
Department of Physics
Period: 01/01/1993 → 14/09/1994
Number of participants: 3
Phd Student:
Offersgaard, Jesper Falden (Intern)
Main Supervisor:
Skettrup, Torben (Intern)
Examiner:
Leistiko, Otto (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-Su Stipendium, Eksperiment
Project: PhD
Investigation of diamond/diamond-like films and buffer layers by x-ray and neutron scattering

Department of Physics
Period: 01/11/1992 → 24/03/1995
Number of participants: 3
Phd Student:
Findeisen, Eberhard (Intern)
Main Supervisor:
Chorkendorff, Ib (Intern)
Examiner:
Hedegård, Per (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Gammel ordning u/skema-SU
Project: PhD

Dynamik i strukturer af Josephson Dioder

Department of Physics
Period: 01/09/1992 → 28/02/1996
Number of participants: 4
Phd Student:
Larsen, Britt Hvolbæk (Intern)
Supervisor:
Samuelsen, Mogens Rugholm (Intern)
Main Supervisor:
Mygind, Jesper (Intern)
Examiner:
Levinsen, Mogens Tveddell (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-stipendium
Project: PhD

Kvanteelektronik og ikke-lineær dynamik

Department of Physics
Number of participants: 2
Phd Student:
Barbara, Paola (Intern)
Main Supervisor:
Mygind, Jesper (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Gammel ordning u/skema-SU
Project: PhD

Transmission electron microscopy investegation of interfaces

Department of Physics
Number of participants: 3
Phd Student:
Mogensen, Kaj Erik (Intern)
Main Supervisor:
Gerward, Leif (Intern)
Examiner:
Johnson, Erik (Intern)
Financing sources
Source: Internal funding (public)
Name of research programme: Centerfinansieret
Project: PhD

Dynamisk simulering af knogleremodellering
Department of Physics
Period: 01/07/1992 → 24/02/1995
Number of participants: 3
PhD Student:
Thomsen, Jesper Skovhus (Intern)
Main Supervisor:
Mosekilde, Erik (Intern)
Examiner:
Colding-Jørgensen, Morten (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Gammel Ordning - Blandet Finan
Project: PhD

Ikke-lineær dynamik i HIV infektion og spredning
Department of Physics
Period: 01/07/1992 → 01/12/1995
Number of participants: 3
PhD Student:
Lund, Ole (Intern)
Main Supervisor:
Mosekilde, Erik (Intern)
Examiner:
Colding-Jørgensen, Morten (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Gammel Ordning - Blandet Finan
Project: PhD

Multiple laserr-inducerede gitter og optiske interconnects i fotorefraktive medier
Department of Physics
Period: 01/03/1992 → 22/06/1995
Number of participants: 3
PhD Student:
Andersen, Peter E. (Intern)
Main Supervisor:
Buchhave, Preben (Intern)
Examiner:
Lading, Lars (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådene via projektbe
Project: PhD

Optiske kommunikationssystemer baseret på solitoner
Department of Physics
Period: 01/03/1992 → 24/03/1995
Number of participants: 2
PhD Student:
**Finansieringskilder**
Source: Internal funding (public)
Name of research programme: Forskerakademiets Samfinansier
Project: PhD

**Fremstilling samt elektrisk og magnetisk undersøgelse af tyndfilm af højtemperatur.**
Department of Physics
Period: 01/02/1992 → 24/03/1995
Number of participants: 4
Phd Student:
Kyhle, Anders (Intern)
Supervisor:
Jacobsen, Claus Schelde (Intern)
Main Supervisor:
Mygind, Jesper (Intern)
Examiner:
Levinsen, Mogens Tveddell (Ekstern)

**Finansieringskilder**
Source: Internal funding (public)
Name of research programme: EF-finansieret
Project: PhD

**Molekylære dynamiksimuleringer i materialvæsnet**
Department of Physics
Period: 01/02/1992 → 22/05/1995
Number of participants: 5
Phd Student:
Schiøtz, Jakob (Intern)
Supervisor:
Nørskov, Jens Kehlet (Intern)
Main Supervisor:
Jacobsen, Karsten Wedel (Intern)
Examiner:
Finnis, Michael William (Ekstern)
Hedegård, Per (Ekstern)

**Finansieringskilder**
Source: Internal funding (public)
Name of research programme: DTU-stipendium
Project: PhD

**Nukleære borehulssonder - konstruktion, målinger og tolkning**
Department of Physics
Period: 01/02/1992 → 05/07/1994
Number of participants: 3
Phd Student:
Poulsen, Anette (Intern)
Main Supervisor:
Øigaard, Povl Lebeck (Intern)
Examiner:
Engstrøm, Finn (Ekstern)

**Finansieringskilder**
Source: Internal funding (public)
Name of research programme: **Særlige grundforskningsfond**
Project: PhD

**Tunnelering og ikke-lineær dynamik i små strukturer**
Department of Physics
Period: 01/02/1992 → 24/03/1995
Number of participants: 4
Phd Student:
Holm (fratrådt), Jesper (Intern)
Supervisor:
Samuelsen, Mogens Rugholm (Intern)
Main Supervisor:
Mygind, Jesper (Intern)
Examiner:
Lindelof, Poul Erik (Intern)

**Financing sources**
Source: Internal funding (public)

Name of research programme: **DTU-stipendium**
Project: PhD

**LIS - New Light Sources, Integrated Optics and Ultrafast Switching**
Department of Physics
Department of Micro- and Nanotechnology
Tele Danmark Research
Aarhus University
Period: 01/01/1992 → 30/11/1996
Number of participants: 2
Project participant:
Skettrup, Torben (Intern)
Project Manager, organisational:
Buchhave, Preben (Intern)

**Financing sources**
Source: Unknown
Name of research programme: **Ukendt**
Amount: 412,000.00 Danish Kroner
Project

**Bifurkationsstrukturer i kobledes ikke-lineære oscillatorer med særlig henblik på biologiske systemer**
Department of Physics
Period: 01/08/1991 → 17/06/1994
Number of participants: 4
Phd Student:
Knudsen, Carsten (Intern)
Supervisor:
Brøns, Morten (Intern)
Main Supervisor:
Mosekilde, Erik (Intern)
Examiner:
Bohr, Tomas (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: **Gammel ordning u/skema-SU**
Materialfysik på paralleldatamater
Department of Physics
Period: 01/08/1991 → 24/03/1995
Number of participants: 4
Phd Student:
Stokbro, Kurt (Intern)
Supervisor:
Nørskov, Jens Kehlet (Intern)
Main Supervisor:
Jacobsen, Karsten Wedel (Intern)
Examiner:
Hedegård, Per (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsstipendium
Project: PhD

Undersøgelser af optiske parametriske oscillatorer (OPOsystemer) specielt mhb anvendelser som infrarøde lyskilder
Department of Physics
Period: 01/07/1991 → 07/04/1995
Number of participants: 3
Phd Student:
Pedersen, Christian (Intern)
Main Supervisor:
Skettrup, Torben (Intern)
Examiner:
Lading, Lars (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: ATV- Gammel ordning
Project: PhD

Brøntproblemer i forbindelse med reaktor havarier
Department of Physics
Period: 01/06/1991 → 21/03/1994
Number of participants: 3
Phd Student:
Bujor, Adrian (Intern)
Main Supervisor:
Ølgaard, Povl Lebeck (Intern)
Examiner:
Thorlaksen, Bjørn (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskerakademiets Samfinansier
Project: PhD

Overfladespektroskopiske undersøgelser af mekanismen ved sammenføjning af metal og keramik
Department of Physics
Period: 01/04/1991 → 08/12/1993
Number of participants: 2
Phd Student:
Alstrup, Niels Christian (Intern)
Main Supervisor:
Chorkendorff, Ib (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: ATV- Gammel ordning
Project: PhD

Studium af ultrasmå magnetiske partikler
Department of Physics
Number of participants: 3
Phd Student:
Bødker, Franz (Intern)
Main Supervisor:
Mørup, Steen (Intern)
Examiner:
Clausen, Bjerne S. (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Gammel ordning u/skema-SU
Project: PhD

Chemisorption of h2 on aluminium and copper surfaces
Department of Physics
Period: 01/02/1991 → ...
Number of participants: 2
Phd Student:
Gundersen, Kent (Intern)
Main Supervisor:
Nørskov, Jens Kehlet (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Gammel ordning u/skema-SU
Project: PhD

Studie af små molekylers vekselvirkning med og reaktioner på - metalkrystaller under UHV med henblik på besk.
Department of Physics
Period: 01/02/1991 → 21/03/1994
Number of participants: 3
Phd Student:
Rasmussen, Peter Bilde (Intern)
Main Supervisor:
Chorkendorff, Ib (Intern)
Examiner:
Hedegård, Per (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Gammel ordning u/skema-SU
Project: PhD

Bioreactor Performance
Department of Physics
Period: 01/10/1990 → 30/05/1994
Number of participants: 3
Conducting Polymers

Polymers with alternating (conjugated) single and double bonds have unusual electronic properties that are normally not associated with polymer materials. By oxidation or reduction, mobile electronic defects may be introduced on the conjugated backbone, rendering these polymers electronic conductors. In extreme cases, electronic conductivity better than copper (by weight!) have been reported. The introduction of charges on the polymer backbone requires that compensating counter charges are introduced into the polymer matrix. This process is often referred to as "doping", but is conceptually identical to an intercalation reaction. Conducting polymers may therefore be useful in the same kind of applications as described above for intercalation materials. We have characterised a number of conducting polymers using the methods developed for characterising intercalation materials and demonstrated how the analogy to intercalation may help in the understanding of the complex behaviour of these systems. One important difference between inorganic intercalation materials and conducting polymers is the lack of perfection of the polymer structure. High concentrations of defects may be present in the chemical bonds making up individual polymer chains, and the stacking of these chains into a "crystal lattice" is far from uniform. By careful control of the synthesis of poly-pyrrole, we have demonstrated how the degree of perfection of the polymer backbone greatly influences the physical and electrochemical properties of the polymer. Polymers are relative soft materials, and the doping process may lead to significant changes in the dimensions of
conducting polymers. We are presently investigating the exploitation of this property in mechanical actuators - "artificial muscles".

Department of Physics
Department of Chemistry
Risø National Laboratory for Sustainable Energy

Danfoss A/S
Period: 01/01/1990 → 31/12/1996
Number of participants: 3
Project participant:
West, Keld (Intern)
Zachau-Christiansen, Birgit (Intern)

Project Manager, organisational:
Skaarup, Steen (Intern)

Project


Department of Physics
Period: 01/08/1989 → 16/08/1995
Number of participants: 2
Phd Student:
Rogaard, Carsten (Intern)
Main Supervisor:
Cotterill, Rodney M J (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Gammel ordning u/skema-SU
Project: PhD

Structure-Property Studies
Many organic compounds have unusual physical properties. For example, they may exhibit high electrical conductivity and in some cases may even become superconductors at very low temperatures. The structures of highly conducting organics typically contain stacks of flat molecules which act as electron donors or acceptors. Conductivity as well as other physical properties are strongly dependent on the actual crystal structure. Organic compounds which are used as molecular dielectric components in devices for pyroelectric detectors, piezoelectric transducers and optical frequency doublers all rely heavily on a non-centrosymmetric crystal structure. Thus, a detailed knowledge of the structural features is essential for systematic studies. Most of the synthetic work takes place at Risø National Laboratory.

Department of Chemistry
Department of Physics
Risø National Laboratory for Sustainable Energy

University of Copenhagen
Period: 01/01/1988 → ...
Number of participants: 5
Project participant:
Krebs, Frederik C (Intern)
Jacobsen, Claus Schelde (Intern)
Bjørnholm, T. (Ekstern)
Bechgaard, Klaus (Intern)

Project Manager, organisational:
Thorup, Niels (Intern)

Project

Varmebehandling af højtømp. superledere samt måling af deres elektriske og magnetiske egenskaber

Department of Physics
Bifurcations in Nephron Pressure and Flow Regulation
Experiments show that the pressure and flow regulation of the functional unit of the kidney (the nephron) can exhibit complex dynamical behaviors. The purpose of the project is to develop a physiologically satisfactory model that can account for clinical observations and reproduce the period-doubling and chaotic dynamics observed under certain circumstances. The characteristic swallow-tail structure of overlapping period-doubling and saddle-node bifurcations is examined by means of one- and two-dimensional bifurcation analyses.

Department of Physics
University of Copenhagen
Period: 01/07/1986 → …
Number of participants: 2
Project participant:
Holstein-Rathlou, Niels-Henrik (Ekstern)
Project Manager, organisational:
Mosekilde, Erik (Intern)

Biomagnetism
Investigation of neural activity in human tissue by means of magnetic measurements using superconducting SQUID sensors.

Department of Physics
Period: 01/06/1981 → …
Number of participants: 4
Project participant:
Kofoed, Bent (Intern)
Pedersen, Jane Rygaard (Intern)
Særmark, Knud (Intern)
Project Manager, organisational:
Bak, Christen Kjeldahl (Intern)

Activities:

A Matter of Relevance: History of technology in High School Education
Period: 13 Jun 2018
Louise Karlskov Skyggebjerg (Other)
Department of Physics
Degree of recognition: International

Related event
Universeum 2018 conference: Working Together: Partnerships, Co-creation, Co-curation
13/06/2018 → 15/06/2018
Glasgow, United Kingdom
Activity: Talks and presentations › Conference presentations
Transmission of information in Thermoacoustic Tomography (TAT)
Period: 5 Jun 2018
Mirza Karamanovic (Guest lecturer)
Department of Applied Mathematics and Computer Science
Scientific Computing
Neutrons and X-rays for Materials Physics
Degree of recognition: International

Related event
SIAM Conference of Imaging Science
05/06/2018 → 08/06/2018
Bologna, Italy
Activity: Talks and presentations › Conference presentations

Corporate environmentalism and the making of environmental knowledge
Period: 24 May 2018
Louise Karskov Skyggebjerg (Speaker)
Department of Physics
Degree of recognition: National

Related event
Dasts 2018
24/05/2018 → 25/06/2018
København, Denmark
Activity: Talks and presentations › Conference presentations

Active-subspace Analysis of Up-crossing Probability for Shallow-water Model
Period: 17 Apr 2018
Kenan Sehic (Guest lecturer)
Mirza Karamanovic (Guest lecturer)
Department of Applied Mathematics and Computer Science
Scientific Computing
Neutrons and X-rays for Materials Physics
Degree of recognition: International

Related event
SIAM Conference on Uncertainty Quantification
16/04/2018 → 19/04/2018
Garden Grove, United States
Activity: Talks and presentations › Conference presentations

Den nordiske Industri-, Landbrugs- og Kunstindustri i Kjøbenhavn 1888
Period: 5 Apr 2018
Louise Karskov Skyggebjerg (Lecturer)
Department of Physics
Degree of recognition: National

Related external organisation
IDA - Historisk Teknologi (HITEK)
Kalvebod Brygge 31, 1560, København K, Denmark
Activity: Talks and presentations › Talks and presentations in private or public companies and organisations
Damp, smør og vandlåse. Industri- og forbrugersamfundet i støbeskeen
Period: 10 Mar 2018
Louise Karlskov Skyggebjerg (Lecturer)
Department of Physics
Degree of recognition: National

Related external organisation
Historiske Dage
Store Kirkestræde 1, 4, 1073, København K, Denmark
Activity: Talks and presentations › Talks and presentations in private or public companies and organisations

The Villum Center for the Science of Sustainable Fuels and Chemicals V-SUSTAIN
Period: 7 Mar 2018
Jakob Kibsgaard (Invited speaker)
Department of Physics
Experimental Surface and Nanomaterials Physics
Description
10th Membership Meeting in Green Ship of the Future hosted by The Danish Maritime Authority
Degree of recognition: International

Related external organisation
Green Ship of the Future
Bygningstorvet 116B, 2800, Kgs. Lyngby, Denmark
Activity: Talks and presentations › Talks and presentations in private or public companies and organisations

Active-subspace analysis of speckle patterns
Period: 6 Mar 2018
Mirza Karamehmedovic (Guest lecturer)
Department of Applied Mathematics and Computer Science
Scientific Computing
Neutrons and X-rays for Materials Physics
Degree of recognition: International
Documents:
Schedule_Full

Related event
17th Electromagnetic and Light Scattering Conference, Texas A&M University, College Station, TX, USA
04/03/2018 → 09/03/2018
College Station, United States
Activity: Talks and presentations › Conference presentations

Egg trays, stainless steel and other unnoticed actors
Period: 22 Feb 2018
Louise Karlskov Skyggebjerg (Guest lecturer)
Department of Physics
Degree of recognition: Local

Related external organisation
Centre for Business History, CBS
Porcelænshaven 18, 2000, Frederiksberg, Denmark
Activity: Talks and presentations › Guest lectures, external teaching and course activities at other universities
Monitoring the state of a nuclear fusion plasma - the role of energetic ions
Period: 30 Jan 2018
Jesper Rasmussen (Speaker)
Department of Physics
Plasma Physics and Fusion Energy

Description
Rydberg Seminar at Univ. of Lund, Sweden

Related external organisation
Lund University
Lund, Sweden
Activity: Talks and presentations › Guest lectures, external teaching and course activities at other universities

DANSCLATT Annual meeting 2017
Period: 2017
Martin Meedom Nielsen (Organizer)
Department of Physics
Neutrons and X-rays for Materials Physics

Related event
DANSCLATT Annual meeting 2017
01/06/2017 → 02/06/2017
Odense, Denmark
Activity: Attending an event › Participating in or organising a conference

Dansk Teknologihistorisk Selskab (External organisation)
Period: 2017 → …
Louise Karlskov Skyggebjerg (Chairman)
Department of Physics

Description
Bestyrelsesmedlem siden 2010
Degree of recognition: National

Related external organisation
Dansk Teknologihistorisk Selskab
Activity: Membership › Membership of committees, commissions, boards, councils, associations, organisations, or similar

Edmuse Conference
Period: 2017 → …
Laila Zwisler (Speaker)
Department of Physics

Description
Conference
Degree of recognition: International
Links:
http://edmuse.eu/ (Link to Edmuse project)

Related event
Edmuse Conference: EdMuse project - Education and Museum: Cultural Heritage for science learning
26/06/2017 → 27/06/2017
Rome, Italy
Activity: Talks and presentations › Conference presentations

**Ianügartion of European XFEL**
**Period:** 2017
Martin Meedom Nielsen (Chairman)
Department of Physics
Neutrons and X-rays for Materials Physics

**Description**
Opening address

**Related event**
**Ianügartion of European XFEL**
01/09/2017 → 01/09/2017
Schenefeld, Germany
Activity: Attending an event › Participating in or organising a conference

**proposal review panel (Event)**
**Period:** 2017
Martin Meedom Nielsen (Member)
Department of Physics
Neutrons and X-rays for Materials Physics
Degree of recognition: International

**Related event**
**proposal review panel**
19/10/2017 → 20/10/2017
villigen, Switzerland
Activity: Membership › Membership in review committee

Æggebakker, rustfrit stål og andre oversete aktører - historie i et hverdags- og materialitetsperspektiv
**Period:** 15 Nov 2017
Louise Karlskov Skyggebjerg (Lecturer)
Department of Physics
Degree of recognition: Local

**Related external organisation**
Idéhistorisk Forening
Aarhus
Activity: Talks and presentations › Talks and presentations in private or public companies and organisations

Folkeuniversitets kursus: Katalysatorer afgør den grønne fremtid
**Period:** 7 Nov 2017 → 28 Nov 2017
Jakob Kibsgaard (Guest lecturer)
Christian Danvad Damsgaard (Guest lecturer)
Peter Christian Kjærgaard Vesborg (Guest lecturer)
Sebastian Horch (Guest lecturer)
Anne Kirsten Frederiksen (Other)
Department of Physics
Experimental Surface and Nanomaterials Physics
Center for Electron Nanoscopy
Related external organisation

Folkeuniversitetet i København
Læderstræde 34, 2, 1201, København, Denmark
Activity: Talks and presentations › Talks and presentations in private or public companies and organisations

ITPA Diagnostics Topical Group (External organisation)
Period: 1 Nov 2017
Søren Bang Korsholm (Vice-chairman)
Department of Physics
Plasma Physics and Fusion Energy

Description
Microwave Working Group (MWG) of the ITPA Diagnostics Topical Group
Degree of recognition: International

Related external organisation

ITPA Diagnostics Topical Group
Activity: Membership › Membership of commitees, commissions, boards, councils, associations, organisations, or similar

Energetic particles in burning plasmas
Period: 26 Sep 2017 → 28 Sep 2017
Jesper Rasmussen (Lecturer)
Department of Physics
Plasma Physics and Fusion Energy

Description
PhD lectures given at the 8th Sino-Danish Autumn School on Fusion Plasma Physics and Technology, Beijing, China

Related event

8th Sino-Danish Autumn School on Fusion Plasma Physics and Technology
26/09/2017 → 28/09/2017
Beijing, China
Activity: Talks and presentations › Guest lectures, external teaching and course activities at other universities

Visualizing Catalysts in Action
Period: 25 Sep 2017
Christian Danvad Damsgaard (Invited speaker)
Center for Electron Nanoscopy
DTU Danchip
Department of Physics
Experimental Surface and Nanomaterials Physics

Description
invited talk https://mcm2017.irb.hr/
Degree of recognition: International

Related event

13th Multinational Congress on Microscopy
25/09/2017 → 29/09/2017
Complex Motion in Fluids Summer School
Period: 24 Sep 2017 → 29 Sep 2017
Seyed Saeed Asadzadeh (Participant)
Jens Honore Walther (Participant)
Lasse Tor Nielsen (Participant)
Julia Dölger (Participant)
Thomas Kjørboe (Participant)
Anders Peter Andersen (Participant)
Department of Mechanical Engineering
Fluid Mechanics, Coastal and Maritime Engineering
National Institute of Aquatic Resources
Centre for Ocean Life
Department of Physics
Biophysics and Fluids

Description
The school will consist of 16 lectures in total, given by 8 speakers (90'+60' each), contributed talks, poster sessions and other activities.

Degree of recognition: International
Documents:
Asadzadeh

Related event
Complex Motion in Fluids Summer School
24/09/2017 → 30/09/2017
Cambridge, United Kingdom
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Combining X-ray and Electron Based in situ Characterization of Catalysts
Period: 23 Sep 2017
Christian Danvad Damsgaard (Invited speaker)
Center for Electron Nanoscopy
DTU Danchip
Department of Physics
Experimental Surface and Nanomaterials Physics

Description
invited talk @ https://coex.iom.cnr.it/
Degree of recognition: International

Related event
Combining electrons with X-rays for integrated in-operando experiments
23/09/2017 → 24/09/2017
Trieste, Italy
Activity: Talks and presentations › Conference presentations

Active-subspace analysis of speckle-based characterisation of particle suspensions
Period: 20 Sep 2017
Mirza Karmahmedovic (Guest lecturer)
Related event

Inverse Problems from Theory to Application
19/09/2017 → 21/09/2017
Cambridge, United Kingdom
Activity: Talks and presentations › Conference presentations

Teknik- och vetenskapshistoriska dagar 2017
Period: 20 Sep 2017
Louise Karlskov Skyggebjerg (Speaker)
Department of Physics
Degree of recognition: National
Documents:
Konerenschemaslutgiltig
Abstract_teknikhistoriska
Links:
https://www.tema.liu.se/tema-t/teknikhistoriska-dagar-2017/?l=sv

Related event

Teknik- og vetenskapshistoriska dagar 2017
20/09/2017 → 22/09/2017
Norrköping, Sweden
Activity: Talks and presentations › Conference presentations

The Life of Flow Injection Analysis and Academic Mass Innovation
Period: 1 Sep 2017
Laila Zwisler (Speaker)
Department of Physics

Description
The study I will present has taken its offset in a group of artefacts from the historical collection at the Technical University of Denmark (DTU). The artefacts stem from the emergence of the flow analysis platform FIA and the further development of FIA. At DTU this development started in 1974. A tale of academic innovation between chemical science, industry, engineering academia and political spheres spun from these artefacts. The stories have a number of typical straits of a recent technoscience development in academia and in the talk I will discuss these traits. The people involved had to negotiate their way between the ethos of science, patent systems, the cooperate world and funding systems. A number of coincidences as well as conscious efforts brought FIA forward onto the international scene. The uneven distribution of wealth in this world opened a path for a technology for mass chemical analysis on the cheap. The fight for resources and enrollment was on. Money was not a goal but a means to sustain continued work. Honour, novelty and opportunity were precious commodities. FIA was not an island; others were on the same trail. I will look into how and why it was perceived as new by some and not by others.

Degree of recognition: International

Related event

ICHC International Conference on the History of Chemistry: 11ICHC
29/08/2017 → 29/09/2017
Trondheim, Norway
Activity: Talks and presentations › Conference presentations

Microscopy Conference 2017
Period: 24 Aug 2017
Christian Danvad Damsgaard (Chairman)
Center for Electron Nanoscopy
DTU Danchip
Department of Physics
Experimental Surface and Nanomaterials Physics

Description
co-chairing the MS 6 session Nanoparticles, 2D materials, nanocomposites and catalysts http://www.mc2017.ch/
Degree of recognition: International

Related event

Microscopy Conference 2017
21/08/2017 → 25/08/2017
Lausanne, Switzerland
Activity: Attending an event › Participating in or organising a conference

In situ microscopy of formation of nickel-based bimetallic nanoparticles
Period: 22 Aug 2017
Christian Danvad Damsgaard (Other)
Center for Electron Nanoscopy
DTU Danchip
Department of Physics
Experimental Surface and Nanomaterials Physics

Description
poster presentation http://www.mc2017.ch/
Degree of recognition: International

Related event

Microscopy Conference 2017
21/08/2017 → 25/08/2017
Lausanne, Switzerland
Activity: Talks and presentations › Conference presentations

Nordisk Historikermøde
Period: 17 Aug 2017
Louise Karlskov Skyggebjerg (Speaker)
Department of Physics
Degree of recognition: International
Documents:
Abstract
Links:
http://www.cgs.aau.dk/forskning/konferencer/nhm

Related event

Nordisk historikermøde
15/08/2017 → 18/08/2017
Aalborg, Denmark
Activity: Talks and presentations › Conference presentations

Spatio-temporally resolved in situ transmission electron microscopy of the dynamics of nanostructured materials
Period: 6 Aug 2017 → 10 Aug 2017
Thomas Willum Hansen (Invited speaker)
Pei Liu (Other)  
Jacob Madsen (Other)  
Philomena Schlexer (Other)  
Béla Sebők (Other)  
Jakob Schiøtz (Other)  
Jakob Birkedal Wagner (Other)  
Center for Electron Nanoscopy  
Center for Nanostructured Graphene  
DTU Danchip  
Department of Physics  
Theoretical Atomic-scale Physics

Related event

Microscopy and Microanalysis 2017  
06/08/2017 → 10/08/2017  
St. Louis, United States  
Activity: Talks and presentations › Conference presentations

International Congress of History of Science and Technology (ICHST)  
Period: 29 Jul 2017  
Louise Karlskov Skyggebjerg (Speaker)  
Department of Physics  
Degree of recognition: International  
Documents:  
Abstract  
Links:  
http://www.ichst2017.sbhc.org.br/

Related event

25th International Congress of History of Science and Technology (ICHST)  
23/07/2017 → 29/07/2017  
Rio de Janeiro, Brazil  
Activity: Talks and presentations › Conference presentations

In situ Characterization of Heterogeneous Catalysts  
Period: 11 Jul 2017  
Christian Danvad Damsgaard (Invited speaker)  
Department of Physics  
Center for Electron Nanoscopy  
DTU Danchip  
Experimental Surface and Nanomaterials Physics

Description  
Invited talk  
Degree of recognition: International  
Documents:  
conference abstract for confernce. Fimpart2017  
Links:  
http://www.fimpart.org/2017/wp/

Related event

Frontiers in Materials Processing Applications, Research and Technology: Enabling innovation  
09/07/2017 → 12/07/2017
Bordeaux, France
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
Department of Energy Conversion and Storage
Electrofunctional materials
Department of Micro- and Nanotechnology

**Description**
Collaborative Conference on Materials Research (CCMR) 2017
Documents:
Abstract Korea

**Related external organisation**

**Kwangwoon University**
Korea, Republic of
Activity: Talks and presentations › Conference presentations

**Velocity space tomography: Methods and results**
Period: 16 Jun 2017
Jesper Rasmussen (Speaker)
Department of Physics
Plasma Physics and Fusion Energy

**Related event**

2nd Joint Nordic Fusion Energy Seminar
15/06/2017 → 16/06/2017
Activity: Talks and presentations › Conference presentations

**Protecting the built environment without killing the idea**
Period: 8 Jun 2017
Laila Zwisler (Speaker)
Department of Physics
Often conservation strategies for the built environment advocate focus on architecture and originality and these are interesting features of many university campuses. But this focus could also fossilize the buildings to such an extent, that they cannot support the main activities of a university. If this happens, what have we really kept for the future? A university must live and evolve and the built environment must often change with it. Can we preserve the atmospheres, the lives lived and the purposes of universities as integrated into the built environment. Should conservation focus mainly on the mundane as well as the signs of use and change? Integrating traces of the past into refurbishments and new buildings can be a way forward. But we need to be very vigilant about our choices and the effects of them. There is more at stake than practicalities. The preserved becomes symbolic, often idealized, and affect identities. If houses as Bourdieu claims can make us reproduce patterns of behavior, our conservation strategies carries very deep messages. One message could be that the past and the future are connected at a university.

Degree of recognition: International

Links:
http://www.universeum2017.rect.bg.ac.rs/preliminaryprogram.php (Conference website)

Related event

Universeum Network Meeting: Mobility of University Heritage
08/06/2017 → 10/06/2017
Belgrade, Serbia
Activity: Talks and presentations › Conference presentations

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)
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
Developing Active Sulfide- and Phosphide-based Catalysts for Sustainable Electrochemical Hydrogen Production
Period: 22 May 2017 → 23 May 2017
Jakob Kibsgaard (Invited speaker)
Department of Physics
Experimental Surface and Nanomaterials Physics

Related event
Dansk Fysisk Selskab annual meeting
22/05/2017 → 23/05/2017
Denmark
Activity: Talks and presentations › Conference presentations

The DTU fusor – Fusion power at your fingertips
Period: 22 May 2017
Jesper Rasmussen (Speaker)
Department of Physics
Plasma Physics and Fusion Energy

Related event
Danish Physical Society Annual Meeting 2017
22/05/2017 → 23/05/2017
Activity: Talks and presentations › Conference presentations

Paul Scherrer Institut (External organisation)
Period: Apr 2017
Martin Meedom Nielsen (Participant)
Department of Physics
Neutrons and X-rays for Materials Physics

Description
Swiss Light Source Proposal panel
Degree of recognition: International

Related external organisation
Paul Scherrer Institut
Switzerland
Activity: Membership › Membership in review committee

Interface engineering to boost the open circuit voltage of Cu2ZnSnS4 solar cells
Period: 18 Apr 2017
Andrea Crovetto (Speaker)
Department of Physics
Experimental Surface and Nanomaterials Physics
Silicon Microtechnology

Related event
2017 MRS Spring Meeting
17/04/2017 → 21/04/2017
Phoenix, United States
Activity: Talks and presentations › Conference presentations
**2017 MRS Spring Meeting**
Period: 17 Apr 2017 → 21 Apr 2017
Andrea Crovetto (Speaker)
Department of Physics
Experimental Surface and Nanomaterials Physics
Silicon Microtechnology

**Related event**

**2017 MRS Spring Meeting**
17/04/2017 → 21/04/2017
Phoenix, United States
Activity: Talks and presentations › Conference presentations

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**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.
Emergence of Engineering Academia and the Teaching Practices at DTU
Period: 5 Apr 2017
Laila Zwisler (Speaker)

Department of Physics

Description
When the Danish polytechnical school opened in 1829 under University of Copenhagen basic sciences were given a dominant role. There was an uneasy and debated relationship between basic sciences and technical subjects. In this talk I will look into how the school dealt with this relationship and the practical executive issues up to 1929. Teachers invoked both the theoretical bodies and the methodology of the natural sciences in the creation of engineering knowledge systems reaching beyond fundamental sciences.
Degree of recognition: National

Related external organisation
IMFUFA course, Roskilde (DK)
Activity: Talks and presentations › Guest lectures, external teaching and course activities at other universities

Optical and Hydrodynamic Stretching of Single Cells from Blood
Period: 3 Apr 2017
Kirstine Berg-Sørensen (Speaker)

Department of Physics
Quantum Physics and Information Technology
Degree of recognition: International
Documents:
3pagesummary

Related event
OSA Biophotonics Congress: Optical Trapping Applications 2017: Optics in the Life Sciences
02/04/2017 → 05/04/2017
San Diego, United States
Activity: Talks and presentations › Conference presentations

Goddag - og farvel - til broer
Period: 26 Mar 2017
Laila Zwisler (Speaker)
Jørgen Burchardt (Speaker)
Magnus Heunicke (Speaker)

Department of Physics

Description
Kan historien lære os om hvordan vi skal planlægge store infrastrukturer som forbindelserne over Femern og Kattegat? Jørgen Burchardt, forsker ved Danmarks Tekniske Museum, fortæller om skæbnen for Tscherning's forslag i 1855 i Folketinget om bro over Lillebælt og tunnel under Storebælt. Laila Zwisler fra Teknologihistorie, DTU, diskuterer, hvordan en ingeniørvædskab har udviklet sig for at holde styr på den moderne verden, hvor teknologiske systemer er blevet vores anden natur. Tidligere trafikminister Magnus Heunicke kommenterer og styrer debat fra publikum.
Degree of recognition: National

Related external organisation
Historiske Dage
Store Kirkestræde 1, 4, 1073, København K, Denmark
Activity: Other

Fremtidens katalyse
Period: 20 Mar 2017
Jakob Kibsgaard (Invited speaker)
Jane Hvolbæk Nielsen (Invited speaker)
Department of Physics
Experimental Surface and Nanomaterials Physics
Documents:
SCIENCE_FILM FORUM_2017_PROGRAM

Related event

CPH:DOX - SCIENCE: FILM FORUM
20/03/2017 → …
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

Related event

Workshop for electromechanical and dielectric materials and devices
09/03/2017 → …
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

DTU CEN - Elektronnanoskopi i verdensklassen
Period: 9 Feb 2017
Christian Danvad Damsgaard (Lecturer)
Jakob Birkedal Wagner (Lecturer)
Department of Physics
Center for Electron Nanoscopy
DTU Danchip
Experimental Surface and Nanomaterials Physics

Description
Kom med IDA Mechanical København på besøg hos Center for Elektronnanoskopi (CEN) på DTU og hør hvordan verdens mest avancerede mikroskoper fungerer, og hvordan man kan se noget, der er mindre end lysets bølgelængde.

CEN blev indviet i december 2007 og er et af verdens mest avancerede laboratorier for elektronmikroskopi. Centeret råder over både skanning elektron mikroskoper (SEM) og transmission elektron mikroskoper (TEM), og mikroskopene er hver i særlig udstyret med yderligere udstyr der fx gør det muligt at bearbejde prøverne med en ion stråle eller nedfrosset kryogen tilstand.

Program:
IDA Mechanical, København, inviterer til en spændende aften hos Center for Elektronnanoskopi (CEN) på DTU, hvor vi får:
• En introduktion til centerets og dets historie
• En beskrivelse af de otte elektronmikroskoper, og hvad de hver især kan benyttes til
• Et overblik over hvilken forskning centeret arbejde med, og hvorfor det er så vigtigt, at kunne undersøge prøver på nanoskala.
• En rundvisning på faciliteterne.
Degree of recognition: Local

Related external organisation
European XFEL user meeting
Period: 24 Jan 2017
Martin Meedom Nielsen (Chairman)
Department of Physics
Neutrons and X-rays for Materials Physics

Description
Opening Address

Related event
European XFEL user meeting
24/01/2017 → 27/01/2017
Activity: Attending an event › Participating in or organising a conference

V-SUSTAIN
Period: 17 Jan 2017
Jakob Kibsgaard (Participant)
Claudie Roy (Participant)
Ib Chorkendorff (Participant)
Department of Physics
Experimental Surface and Nanomaterials Physics

Description
Interview on The Villum Center for the Science of Sustainable Fuels and Chemicals (V-SUSTAIN)

Related external organisation
filmbureauet ApS
c/o Freezone. Rosenborggade 17, 1130, København K., Denmark

Activity: Other

67th Annual Meeting of the International Society of Electrochemistry
Period: 2016 → …
Brian Seger (Organizer)
Department of Physics
Experimental Surface and Nanomaterials Physics

Description
Symposium Organizer (Symposium #18)

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: Attending an event › Participating in or organising a conference

Summer School- DTU CINF 2016
Period: 2016
Brian Seger (Organizer)
Department of Physics
Experimental Surface and Nanomaterials Physics

Description
Organizing Committee Member

Related event

Summer School- DTU CINF 2016: Reactivity of nanoparticles for more efficient and sustainable energy conversion: Rising technologies
07/08/2016 → 12/12/2016
Gilleleje, Denmark
Activity: Attending an event › Participating in or organising a conference

Kemi og akademisk innovation
Period: 2 Dec 2016
Laila Zwisler (Speaker)
Department of Physics

Description

Filmen er en del af et undervisningsmateriale fra Teknologihistorie DTU til gymnasiet om kemi, historie og etik:
http://www.historie.dtu.dk/formidling....

Projektet er støttet af Uddannelses- og Forskningsministeriets Udlodningsmidler.
Degree of recognition: Local
Links:
hhttps://www.youtube.com/watch?v=MNZGvI8koaQ

Related organisation

Kemi og akademisk innovation
Zwisler, L. (Speaker)
2 Dec 2016
Activity: Talks and presentations › Talks and presentations in private or public companies and organisations

Kulturstudier (Journal)
Period: Nov 2016 → …
Louise Karlskov Skyggebjerg (Editor)
Department of Physics

Description
Dansk tidskrift for kulturhistorie, etnologi, folkloristik og lokalhistorie

Medlem af redaktionen

Related journal

Kulturstudier
Indexed in DOAJ
Local database
Activity: Research › Journal editor

ATV Sustain conference
Period: 30 Nov 2016
Søren Bang Korsholm (Speaker)
Department of Physics
Plasma Physics and Fusion Energy

**Description**
Poster and poster pitch talk: Developing diagnostic systems for ITER – the next step fusion energy experiment

Poster presentation of "Developing diagnostic systems for ITER – the next step fusion energy experiment"
Links:
http://www.sustain.dtu.dk/ (Conference website)

**Related event**

**ATV Sustain conference**
30/11/2016 → 30/11/2016
Activity: Talks and presentations › Conference presentations

**Sustainable Electrochemical Hydrogen Production**
Period: 30 Nov 2016
Jakob Kibsgaard (Speaker)
Department of Physics
Experimental Surface and Nanomaterials Physics
Documents:
Sustain2016abstract_JakobKibsgaard
Links:
http://www.sustain.dtu.dk/

**Related event**

**Sustain-ATV Conference 2016**
30/11/2016 → 30/11/2016
Kgs. Lyngby, Denmark
Activity: Talks and presentations › Conference presentations

**Hydrodynamics of Microbial Filter-Feeding**
Period: 21 Nov 2016
Anders Peter Andersen (Lecturer)
Department of Physics
Biophysics and Fluids
Links:
http://meetings.aps.org/Meeting/DFD16/Session/H39.7

**Related external organisation**

**Unknown external organisation**
Activity: Talks and presentations › Conference presentations

**PhD Defense Opponent (External organisation)**
Period: 14 Oct 2016
Brian Seger (External examiner)
Department of Physics
Experimental Surface and Nanomaterials Physics

**Description**
I was a PhD Defense Opponent for Moreno de Respinis from TU Delft
Degree of recognition: International
Activity: Examinations and supervision › External examination
Address at the inauguration of the European XFEL Head Quarters, Schenefeld campus, Schenefeld, Germany
Period: 6 Oct 2016
Martin Meedom Nielsen (Chairman)
Department of Physics
Neutrons and X-rays for Materials Physics

Description
Address at the inauguration of the European XFEL Head Quarters
Address at the inauguration of the European XFEL Head Quarters, Schenefeld campus, Schenefeld, Germany
Address at the inauguration of the European XFEL Head Quarters, Schenefeld campus, Schenefeld, Germany

Related event
Address at the inauguration of the European XFEL Head Quarters, Schenefeld campus, Schenefeld, Germany
06/10/2016 → …
Schenefeld, Germany
Activity: Attending an event › Participating in or organising a conference

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

Diagnosing fusion-born alpha particles in ITER (and DEMO?)
Period: 26 Sep 2016 → 30 Sep 2016
Jesper Rasmussen (Lecturer)
Department of Physics
Plasma Physics and Fusion Energy

Description
PhD lectures given at the 7th Sino-Danish Autumn School on Fusion Plasma Physics and Technology, Hefei, China

Related event
7th Sino-Danish Autumn School on Fusion Plasma Physics and Technology
26/09/2016 → 30/09/2016
Hefei, China
Activity: Talks and presentations › Guest lectures, external teaching and course activities at other universities

Vær Forberedt
Period: 22 Sep 2016
Laila Zwisler (Speaker)
Department of Physics

Description
Når krisen kradser kommer teknologiudvikling i spil! 1970’erne var skelsættende år, hvor danskerne udskiftede 50’ernes og 60’ernes vækstoptimisme med pessimisme. Oliekriser og miljøproblemer pustede for alvor liv i debatten om det moderne samfunds sårbarhed. Golden Days temaet i år har fokus på 1970’ernes modsætninger og de mødes også i
denne udstilling. Protestbevægelser og velfærdssat mødte den ansigtsløse kolde krig. Angsten for atomkrig smeltede sammen med modstanden mod det etablerede samfund og skepsis overfor teknologi. Hvad var den teknologiske respons på alt dette? Var det rationelle løsninger eller et sted at parkere vores angst? Og har det egentlig noget at gøre med det sagnomspundne tunnelsystem under DTU?

Laila Zwisler er arrangementets verbale tour-guide i dette spændende og alsidige oplæg om at være forberedt og nogle af de sære veje teknologien kan tage.

Related external organisation

DTU Bibliotek
Activity: Talks and presentations › Talks and presentations in private or public companies and organisations

Efteruddannelseskursus i plasmafysik og fusion
Period: 19 Sep 2016
Søren Bang Korsholm (Organizer)
Department of Physics
Plasma Physics and Fusion Energy

Description
Kursusplanlægger sammen med LMFK, samt oplægsholder med et fusionsroadshow
Links:
https://www.lmfk.dk/index.phtml?sek_id=11&con_id=716

Related event

Efteruddannelseskursus i plasmafysik og fusion: LMFK/DTU arrangeret kursus
19/09/2016 → 20/09/2016
Lyngby, Denmark
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Koordinator og kulturhistorie: Fra historisk GIS til Spatial Humanities
Period: 14 Sep 2016
Louise Karlskov Skyggebjerg (Speaker)
Department of Physics

Description
Poster: Leg med hele Danmarks befolkning

Related event

Koordinator og kulturhistorie: Fra historisk GIS til Spatial Humanities
14/09/2016 → …
Odense, Denmark
Activity: Talks and presentations › Conference presentations

Kursus i plasmafysik og fusion
Period: 8 Sep 2016
Søren Bang Korsholm (Organizer)
Department of Physics
Plasma Physics and Fusion Energy

Description
Kursusplanlægger sammen med LMFK, samt oplægsholder med et generelt fusionsforskningsforedrag
Links:
https://www.lmfk.dk/index.phtml?sek_id=11&con_id=716
Related event

Kursus i plasmafysik og fusion: Århus: LMFK/DTU arrangeret efteruddannelse
08/09/2016 → 09/09/2016
Aarhus, Denmark
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

21st EU-US Transport Task Force Meeting, Leysin, Switzerland 5-8 September 2016
Period: 5 Sep 2016 → 8 Sep 2016
Jens Juul Rasmussen (Lecturer)
Department of Physics
Plasma Physics and Fusion Energy
Description
Oral Contribution:
Simulations of filamentary transport in the SOL and estimations of the power deposition profile
Documents:
TTF-2016_SOL_transport_Rasmussen

Related external organisation

Unknown external organisation
Activity: Talks and presentations › Conference presentations

Optical manipulation with two beam traps in microfluidic polymer systems
Period: 30 Aug 2016
Kirstine Berg-Sørensen (Invited speaker)
Department of Physics
Biophysics and Fluids
Description
Inviteret foredrag ved "Optical Trapping and Optical Micromanipulation" XIII, SPIE Optics and Photonics 2016

Related external organisation

Unknown external organisation
Activity: Talks and presentations › Conference presentations

Dansk Historikermøde 2016
Period: 26 Aug 2016
Louise Karlskov Skyggebjerg (Speaker)
Department of Physics
Description
Erfervshistorie og den materielle vending
Degree of recognition: National

Related event

Dansk Historikermøde 2016
26/08/2016 → 27/08/2016
Odense, Denmark
Activity: Talks and presentations › Conference presentations

67th Annual Meeting of the International Society of Electrochemistry in The Hague
Heine Anton Hansen (Speaker)

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

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
12/08/2016 → …
Pittsburgh, United States
Activity: Talks and presentations › Guest lectures, external teaching and course activities at other universities

Modeling of Tandem Devices for Photoelectrochemical CO2 Reduction
Period: 28 Jul 2016
Brian Seger (Lecturer)
Department of Physics
Experimental Surface and Nanomaterials Physics

Description
Oral Lecture

Related event

21st International Conference on Photochemical Conversion and Storage of Solar Energy
25/07/2016 → 29/07/2016
Saint Petersburg, Russian Federation
Activity: Talks and presentations › Conference presentations

Intragranular orientation spread induced by grain interaction
Period: 12 Jul 2016
Jette Oddershede (Lecturer)
Department of Physics
Neutrons and X-rays for Materials Physics

Related event
3rd International Congress on Materials Science  
10/07/2016 → 13/07/2016  
St. Charles, United States  
Activity: Talks and presentations › Conference presentations  

ICOM general conference  
Period: 5 Jul 2016  
Laila Zwisler (Speaker)  
Department of Physics  

Description  
UNIVERSITY CAMPUS AND COLLECTIONS COMBINING AS A CULTURAL LANDSCAPE – NUDGING AND CRITICAL THINKING  

ICOM 24th General Conference Milano 2016  
Documents:  
ZwislerSorensenLanngDTU  

Related event  
ICOM general conference: Museums and cultural landscapes  
03/07/2016 → 09/07/2016  
Milano, Italy  
Activity: Talks and presentations › Conference presentations  

Mathematics Working Group of the European Society for Engineering Education (External organisation)  
Mirza Karamemehedovic (Participant)  
Department of Applied Mathematics and Computer Science  
Scientific Computing  
Neutrons and X-rays for Materials Physics  

Description  
National contact point for Denmark  
Degree of recognition: International  

Related external organisation  
Mathematics Working Group of the European Society for Engineering Education  
Activity: Membership › Membership of committees, commissions, boards, councils, associations, organisations, or similar  

Critical Edge Alliance Conference 2016  
Period: 24 Jun 2016  
Laila Zwisler (Speaker)  
Department of Physics  

Description  
Dealing with the unknown in early Scientific Engineering education  

Critical Edge Alliance Conference 2016  
Documents:  
8DealingWithUnknown  

Related event  
Critical Edge Alliance Conference 2016: Innovative and Critical Approaches to Higher Education in the 21st Century  
22/06/2016 → 24/06/2016  
Roskilde, Denmark  
Activity: Talks and presentations › Conference presentations
Society for the History of Technology
Period: 24 Jun 2016
Louise Karlskov Skyggebjerg (Speaker)
Department of Physics

Description
Thinking with objects

Related event
Society for the History of Technology: Annual Meeting 2016
22/06/2016 → 26/06/2016
Singapore, Singapore
Activity: Talks and presentations › Conference presentations

Chemical Dynamics in an X-ray Scattering Perspective
Period: 14 Jun 2016
Martin Meedom Nielsen (Keynote speaker)
Department of Physics
Neutrons and X-rays for Materials Physics

Related event
Research Opportunities in Photochemistry, Solar Energy & Advanced X-ray Methods
14/06/2016 → 17/06/2016
Menlo Park, United States
Activity: Talks and presentations › Conference presentations

Universeum Network Meeting
Period: 9 Jun 2016
Laila Zwisler (Speaker)
Department of Physics
TechnologicalHistory•DTU

Description
Do Connections Require Wired People

Related event
Universeum Network Meeting: Connecting Collections
09/06/2016 → 11/06/2016
Amsterdam, Netherlands
Activity: Talks and presentations › Conference presentations

Grain-scale investigations of deformation and surface treatment of stainless steel
Period: 8 Jun 2016
Jette Oddershede (Lecturer)
Department of Physics
Neutrons and X-rays for Materials Physics

Description
CHESS-U: New Industrial and Scientific Opportunities for Structural Materials: Data, Modeling, Manufacturing

Related external organisation
Hot enough for you? Monitoring the health of a nuclear fusion plasma  
**Period:** 6 Jun 2016 → 7 Jun 2016  
**Jesper Rasmussen (Speaker)**  
Department of Physics  
Plasma Physics and Fusion Energy  

**Description**  
Contributed talk, Danish Physical Society Annual Meeting 2016, Middelfart, Denmark. Awarded "Best Talk" at the meeting.

Photocatalytic water splitting- The advantages of using a 2-photon tandem approach  
**Period:** 6 Jun 2016  
**Brian Seger (Invited speaker)**  
Department of Physics  
Experimental Surface and Nanomaterials Physics

**Related event**  
Dansk Fysisk Selskab Årsmøde 2016  
06/06/2016 → 07/06/2016  
Middelfart, Denmark

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

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

Curatorial Challenges
Period: 26 May 2016 → 27 May 2016
Laila Zwisler (Participant)
Department of Physics
TeknologiHistorie DTU

Description
Curatorial Challenges

Related event

Curatorial Challenges
26/05/2016 → 27/05/2016
Copenhagen, Denmark
Activity: Attending an event › Participating in or organising a conference

Exploring optical manipulation in and of cells
Period: 17 May 2016
Kirstine Berg-Sørensen (Speaker)
Department of Physics
Biophysics and Fluids
Degree of recognition: International

Related external organisation

Academy of Sciences of the Czech Republic
Czech Republic
Activity: Talks and presentations › Conference presentations

Fast Physical Processes studied at XFELs, Dynamic Structural Science Workshop, Cosener's House, Abingdon, UK
Period: 25 Apr 2016
Martin Meedom Nielsen (Invited speaker)
Department of Physics
Neutrons and X-rays for Materials Physics

Related event

Dynamic Structural Science Workshop
Oxford, United Kingdom
Activity: Talks and presentations › Guest lectures, external teaching and course activities at other universities

HD-Tomo Days
Period: 6 Apr 2016 → 8 Apr 2016
Mirza Karamemhedovic (Participant)
Department of Applied Mathematics and Computer Science
Scientific Computing
Neutrons and X-rays for Materials Physics
HD-Tomo Days

Related event

HD-Tomo Days
06/04/2016 → 08/04/2016
Kgs. Lyngby, Denmark
Activity: Attending an event › Participating in or organising a conference

SIAM Conference on Uncertainty Quantification
Period: 5 Apr 2016 → 8 Apr 2016
Magnus Dam (Participant)
Department of Applied Mathematics and Computer Science
Mathematics
Plasma Physics and Fusion Energy

Description
Participation in conference

Related event

SIAM Conference on Uncertainty Quantification
05/04/2016 → 08/04/2016
Lausanne, Switzerland
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Electronic and Structural Dynamics in Solvated Metal Complexes Enlightened by XFEL Experiments, Workshop to Define the Science Case for a Soft X-ray Laser Beamline at MAX IV, Stockholm, SE
Period: 21 Mar 2016
Martin Meedom Nielsen (Invited speaker)
Department of Physics
Neutrons and X-rays for Materials Physics

Related event

Electronic and Structural Dynamics in Solvated Metal Complexes Enlightened by XFEL Experiments, Workshop to Define the Science Case for a Soft X-ray Laser Beamline at MAX IV, Stockholm, SE
21/03/2016 → 21/03/2016
Stockholm, Sweden
Activity: Talks and presentations › Conference presentations

Ecole Polytechnique Federale de Lausanne (EPFL)
Magnus Dam (Visiting researcher)
Department of Applied Mathematics and Computer Science
Mathematics
Plasma Physics and Fusion Energy

Description
Research Stay at EPFL
An external stay at the Mathematics Institute of Computational Science and Engineering (MATHICSE) at École Polytechnique Fédérale de Lausanne. Performed work on PhD project supervised by Professor Jan Hesthaven.
Activity: Visiting an external institution › Visiting another research institution
Inverse scattering problems in characterisation of nanomaterials
Period: 11 Feb 2016
Mirza Karamehmedovic (Invited speaker)
Department of Applied Mathematics and Computer Science
Scientific Computing
Neutrons and X-rays for Materials Physics

Description
Inverse scattering problems in characterisation of nanomaterials
Degree of recognition: International

Related event
Inverse scattering problems in characterisation of nanomaterials
11/02/2016 → ...
Sarajevo, Bosnia and Herzegovina
Activity: Talks and presentations › Guest lectures, external teaching and course activities at other universities

Visualizing Structural Dynamics in Solvated Metal Complexes by XFEL Experiments, 7th Ringberg Workshop on Science with FELs - from first results to future perspectives, Ringberg, Germany
Period: 8 Feb 2016
Martin Meedom Nielsen (Invited speaker)
Department of Physics
Neutrons and X-rays for Materials Physics

Description
Visualizing Structural Dynamics in Solvated Metal Complexes by XFEL Experiments, 7th Ringberg Workshop on Science with FELs - from first results to future perspectives, Ringberg, Germany

Related event
Visualizing Structural Dynamics in Solvated Metal Complexes by XFEL Experiments, 7th Ringberg Workshop on Science with FELs - from first results to future perspectives, Ringberg, Germany
08/02/2016 → 10/02/2016
Ringberg, Germany
Activity: Talks and presentations › Guest lectures, external teaching and course activities at other universities

European XFEL users meeting
Period: 27 Jan 2016
Martin Meedom Nielsen (Invited speaker)
Department of Physics
Neutrons and X-rays for Materials Physics

Description
Opening Address, XFEL.EU users meeting, Hamburg, Germany.

Related event
European XFEL users meeting
27/01/2016 → 29/01/2016
Hamburg, Germany
Activity: Talks and presentations › Conference presentations
Danish Instruments for Big Science 2016
Period: 25 Jan 2016
Søren Bang Korsholm (Organizer)
Department of Physics
Plasma Physics and Fusion Energy

Description
In the central organising committee of DIBS’16

DIBS is an annually recurring conference, which gathers together universities and businesses with experience in or interest in delivering instruments for large research infrastructure, so called Big Science facilities. Taking on instruments for Big Science facilities relies on high level competence- and technology development, potentially to the benefit of both academia and businesses alike. The objective of DIBS is to strengthen the exchanges going on between these and to ensure a more efficient build up process as well as an increase of Danish deliveries of high quality instruments in the future.

Links:
http://www.nbi.ku.dk/english/calendar/activities_16/danish_instruments_big_science/tilmelding/ (Conference link)

Related event

Danish Instruments for Big Science 2016
25/01/2016 → 25/01/2016
København, Denmark
Activity: Attending an event › Participating in or organising a conference

Materials characterisation tools towards lead-free piezoceramics
Period: 17 Dec 2015
Jette Oddershede (Lecturer)
Department of Physics
Neutrons and X-rays for Materials Physics

Related event

DTU Sustain Conference 2015
17/12/2015 → 17/12/2015
Lyngby, Denmark
Activity: Talks and presentations › Conference presentations

Quiet swimming at low Reynolds number
Period: 23 Nov 2015
Anders Peter Andersen (Lecturer)
Department of Physics
Biophysics and Fluids
Links:
http://meetings.aps.org/Meeting/DFD15/Session/H25.3

Related external organisation

Unknown external organisation
Activity: Talks and presentations › Conference presentations

Kultur- og naturhistorisk orienteringsmøde
Period: 17 Nov 2015
Louise Karlskov Skyggebjerg (Speaker)
Department of Physics

Description
Indlæg: Har du talt med dine genstande i dag?
Related event

Kultur- og naturhistorisk orienteringsmøde: Arrangeret af Organisationen Danske Museer (ODM)
16/11/2015 → 18/11/2015
Kolding, Denmark
Activity: Talks and presentations › Conference presentations

Optical Manipulation with Two Beam Traps in Microfluidic Polymer Systems
Period: 26 Oct 2015
Kirstine Berg-Sørensen (Invited speaker)
Department of Physics
Biophysics and Fluids
Description
Inviteret foredrag ved MOC’15, Japan, Oktober 2015

Related external organisation

Unknown external organisation
Activity: Talks and presentations › Conference presentations

Quantitative grain-scale ferroelectric domain volume fractions and domain switching strains measured by 3DXRD during in situ electrical poling
Period: 1 Oct 2015
Jette Oddershede (Lecturer)
Department of Physics
Neutrons and X-rays for Materials Physics

Related event

8th International Conference on Mechanical Stress Evaluation by Neutron and Synchrotron Radiation
30/09/2015 → 02/10/2015
Grenoble, France
Activity: Talks and presentations › Conference presentations

DTU Cen World Class Electron Microscopy
Period: 24 Sep 2015
Christian Danvad Damsgaard (Lecturer)
Jakob Birkedal Wagner (Speaker)
Center for Electron Nanoscopy
DTU Danchip
Department of Physics
Experimental Surface and Nanomaterials Physics
Description
Public lecture in IDA M regarding DTU Cen and electron microscopy
Links:
https://ida.dk/event/314993

Related external organisation

The Danish Society of Engineers, IDA
Kalvebod Brygge 31-33, DK-1780, Copenhagen V, Denmark
Activity: Talks and presentations › Talks and presentations in private or public companies and organisations

Polymer injection molding of hard X-ray refractive optics
Period: 24 Sep 2015
Frederik Stöhr (Speaker)
DTU Danchip
Neutrons and X-rays for Materials Physics

**Related event**

41st International conference on Micro and Nano Engineering : MNE 2015  
21/09/2015 → 24/09/2015  
The Hague, Netherlands  
Activity: Talks and presentations › Conference presentations

23rd International Congress on X-ray Optics and Microanalysis  
Period: 14 Sep 2015 → 15 Sep 2015  
Frederik Stöhr (Participant)
DTU Danchip
Neutrons and X-rays for Materials Physics

**Description**
Poster Presentation
Microfabrication and testing of refractive hard X-ray optics

**Related event**

23rd International Congress on X-ray Optics and Microanalysis  
14/09/2015 → 18/09/2015  
Upton, New York, United States  
Activity: Attending an event › Participating in or organising a conference

Fast ion properties in fusion plasmas: Theory and measurements  
Period: 14 Sep 2015 → 18 Sep 2015  
Jesper Rasmussen (Lecturer)
Department of Physics
Plasma Physics and Fusion Energy

**Description**
PhD lectures given at the 6th Sino-Danish Autumn School on Fusion Plasma Physics and Technology, Hefei, China

**Related event**

6th Sino-Danish Autumn School on Fusion Plasma Physics and Technology  
14/09/2015 → 18/09/2015  
Hefei, China  
Activity: Talks and presentations › Guest lectures, external teaching and course activities at other universities

Dynamics Days Europe 2015  
Period: 6 Sep 2015 → 10 Sep 2015  
Magnus Dam (Participant)
Department of Applied Mathematics and Computer Science
Mathematics
Department of Physics
Plasma Physics and Fusion Energy

**Description**
Attended conference and presented a poster.
Documents:
Investigating fast-ion transport due to sawtooth crashes using Collective Thomson Scattering
Period: 31 Aug 2015 → 4 Sep 2015
Jesper Rasmussen (Speaker)
Department of Physics
Plasma Physics and Fusion Energy

Description
Contributed talk, 14th IAEA Technical Meeting on Energetic Particles in Magnetic Confinement Systems, Vienna, Austria

Related external organisation
Unknown external organisation
Activity: Talks and presentations › Conference presentations

The International Committee for the History of Technology
Period: 19 Aug 2015
Louise Karlskov Skyggebjerg (Speaker)
Department of Physics

Description
Paper: World War I and cross-country transfer of high technologies

Related event
The International Committee for the History of Technology: History of High-Technologies and Their Socio-Cultural Contexts. Annual Meeting 2015
16/08/2015 → 21/08/2015
Tel Aviv, Israel
Activity: Talks and presentations › Conference presentations

Fusionsenergi - efterligning af stjernernes energikilde
Period: 29 Jul 2015
Jesper Rasmussen (Lecturer)
Department of Physics
Plasma Physics and Fusion Energy

Description
Public lecture presented to high-school students at the UNF Fysik Camp 2015

Related external organisation
Unknown external organisation
Activity: Talks and presentations › Talks and presentations in private or public companies and organisations

Plasma transport in the Scrape-off-Layer of magnetically confined plasma and the plasma exhaust
Period: 26 Jul 2015 → 31 Jul 2015
Jens Juul Rasmussen (Invited speaker)
Department of Physics
Plasma Physics and Fusion Energy

Description
Invited contribution at 32nd International Conference on Phenomena in Ionized Gases - July 26 - 31, 2015 Iasi, Romania

32nd ICPIG, July 26-31, 2015, Iasi, Romania
Documents:
J_J_Rasmussen_Topical_Review

Related external organisation
Unknown external organisation
Activity: Talks and presentations › Conference presentations

Ph.D. School-Conference on "Mathematical Modeling of Complex Systems"
Magnus Dam (Participant)
Department of Applied Mathematics and Computer Science
Mathematics
Department of Physics
Plasma Physics and Fusion Energy

Description
Course participation

Related event
Ph.D. School-Conference on "Mathematical Modeling of Complex Systems"
20/07/2014 → 30/07/2015
Patras, Greece
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Numerical modelling of the transition from low to high confinement in magnetically confined plasma
Period: 22 Jun 2015 → 26 Jun 2015
Jens Juul Rasmussen (Invited speaker)
Department of Physics
Plasma Physics and Fusion Energy

Description
42nd European Physical Society Conference on Plasma Physics, Lisbon, Portugal, June 2015

42nd European Physical Society Conference on Plasma Physics, Lisbon, Portugal, June 2015
Documents:
Abstract_EPS_15_J_Juul_Rasmussen

Related external organisation
Unknown external organisation
Activity: Talks and presentations › Conference presentations

Summer School on Quantum and Nonlinear Optics 2015
Period: 7 Jun 2015 → 13 Jun 2015
Andreas Dyhl Østerkryger (Participant)
Department of Photonics Engineering
Department of Physics
Nanophotonics Theory and Signal Processing
Description
Participation in summer school on quantum and nonlinear optics (QNLO) 2015.
Links:
http://www.fysik.dtu.dk/english/Research/QPIT/Events/Summer_school_2015

Related event

Quantum and Nonlinear Optics. PhD Summer School, 2015
07/06/2015 → 13/06/2015
Ringsted, Denmark
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Ting, teknologi og industri
Period: 29 May 2015
Louise Karlskov Skyggebjerg (Organizer)
Department of Physics

Description
Indlæg: Hvad er ting? Og hvad skal vi med dem?

Related event

Ting, teknologi og industri: Industripuljemøde / Årsmøde i Dansk Teknologihistorisk Selskab
29/05/2015 → 30/05/2015
Helsingør, Denmark
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

MyFab-NorFab meeting 2015
Period: 21 Apr 2015 → 22 Apr 2015
Frederik Stöhr (Participant)
DTU Danchip

Neutrons and X-rays for Materials Physics

Description
Poster presentation on recent progress in silicon hard X-ray lens development at DTU Danchip.
X-ray refractive optics. Manufacture, shape characterization and optical performance.
Documents:
Poster
Links:
http://www.myfab.se/Start/MyfabUserMeeting.aspx (Myfab and NorFab User Meeting 2015)

Related event

MyFab-NorFab meeting 2015
21/04/2015 → 22/04/2015
Lund, Sweden
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Teknik- och vetenskapshistoriska dagar
Period: 16 Apr 2015
Louise Karlskov Skyggebjerg (Speaker)
Department of Physics

Description
Paper: Ting som historiefortællere

Related event

Teknik- och vetenskapshistoriska dagar
2nd Optical Nanospectroscopy Conference
Marta Espina Palanco (Participant)
Department of Physics
Biophysics and Fluids

Description
SERS sensing of plant materials
M. Espina Palanco (1), K. Bo Mogensen (2), K. Kneipp (1)
Danmarks Tekniske Universitet DTU, (1) Department of Physics and (2) Department of Micro- and Nanotechnology. 2800 Kgs. Lyngby, Denmark
Documents:
Abstract_Marta_espina

Related event
2nd Optical Nanospectroscopy Conference
18/03/2015 → 20/03/2015
Dublin, Ireland
Activity: Attending an event › Participating in or organising a conference

Three-Dimensional X-ray Diffraction (3DXRD) microscopy for in situ studies of polycrystalline materials
Period: 16 Mar 2015
Jette Oddershede (Lecturer)
Department of Physics
Neutrons and X-rays for Materials Physics

Description
Polycrystalline Materials: Bringing Together Experiments, Simulations, and Analytical Theories, invited presentation.

Related event
TMS 2015 Annual Meeting & Exhibition
15/03/2015 → 19/03/2015
Orlando, FL, United States
Activity: Talks and presentations › Conference presentations

Hvem var Ole Opfinder?
Period: 14 Mar 2015
Laila Zwisler (Speaker)
Department of Physics

Description
Med opfindelser skal land bygges.

Related event
Historiske Dage 2015
14/03/2015 → 15/03/2015
Copenhagen, Denmark
Activity: Talks and presentations › Conference presentations

Chair of the Search and Selection Committee XFEL. EU (External organisation)
Martin Meedom Nielsen (Chairman)
Department of Physics
Neutrons and X-rays for Materials Physics

**Description**
Chair of the Search and Selection Committee for the Chairperson of the Management Board, XFEL. EU
Degree of recognition: International

**Related external organisation**
Chair of the Search and Selection Committee XFEL. EU
Activity: Membership › Membership of committees, commissions, boards, councils, associations, organisations, or similar

**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.

4th Annual Niels Bohr International Academy Workshop-School on ESS Science
Period: 10 Nov 2014 → 14 Nov 2014
Ellen Fogh (Participant)
Department of Physics
Neutrons and X-rays for Materials Physics

**Description**
This year our workshop-school is intended to be a forum of discussion of how the use of X-ray and neutron reflectometry tells us about the binding of molecules to a surface and of how the characteristic frequencies of motions of surface-bound molecules can be detected by inelastic neutron scattering, and finally, how such experimental results can be interpreted by molecular dynamics simulations.
Documents:
highFieldPoster

**Related event**
4th Annual Niels Bohr International Academy Workshop-School on ESS Science
10/11/2014 → 14/11/2014
Copenhagen, Denmark
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

4th Annual Niels Bohr International Academy Workshop-School on ESS Science
Period: 10 Nov 2014 → 14 Nov 2014
Alberto Cereser (Participant)
Department of Physics
Neutrons and X-rays for Materials Physics
Documents:
Poster NBIA workshop
**Related event**

4th Annual Niels Bohr International Academy Workshop-School on ESS Science  
10/11/2014 → 14/11/2014  
Copenhagen, Denmark  
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

**Magnetic High-Field Phases of Magnetoelectric LiNiPO4**  
Period: 30 Oct 2014  
Ellen Fogh (Speaker)  
Department of Physics  
Neutrons and X-rays for Materials Physics  

**Description**  
The scope of the workshop is to bring together experts doing research in high magnetic fields above 15 T with the focus on neutron scattering. We want to provide an information platform for researchers regarding the future use of the high-field facility capable to generate magnetic fields as high as 25+ T at HZB. Identification of possible future experiments using this facility is one of the main workshop topics. The workshop covers a broad field of topics ranging from the neutron diffraction and scattering in high magnetic fields and sample environment for neutron sciences up to fundamental physics problems in high magnetic fields.  
Documents:  
abstract_hfm_workshop_EllenFogh

**Related event**

Neutron Scattering in Magnetic Fields Above 15 Tesla  
29/10/2014 → 30/10/2014  
Berlin, Germany  
Activity: Talks and presentations › Conference presentations

**World Conference on Neutron Radiography**  
Alberto Cereser (Participant)  
Department of Physics  
Neutrons and X-rays for Materials Physics  
Documents:  
Poster WCNR 2014

**Related event**

World Conference on Neutron Radiography  
05/10/2014 → 10/10/2014  
Grindewald, Switzerland  
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

**Three-Dimensional X-ray Diffraction (3DXRD) microscopy for studying strain evolution in piezoelectric domain structures and deformation induced twinning**  
Period: 30 Sep 2014  
Jette Oddershede (Lecturer)  
Department of Physics  
Neutrons and X-rays for Materials Physics

**Related event**

Nordic X-ray Science Days  
29/09/2014 → 01/10/2014  
Lund, Sweden  
Activity: Talks and presentations › Conference presentations
**Fast ion properties in fusion plasmas: Theory and measurements**

Period: 15 Sep 2014 → 19 Sep 2014

Jesper Rasmussen (Lecturer)

Department of Physics

Plasma Physics and Fusion Energy

**Description**

PhD lectures given at the 5th Sino-Danish Autumn School on Fusion Plasma Physics and Technology, Hefei, China

**Related event**

5th Sino-Danish Autumn School on Fusion Plasma Physics and Technology

15/09/2014 → 19/09/2014

Hefei, China

Activity: Talks and presentations › Guest lectures, external teaching and course activities at other universities

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**Worklab Conference**

Period: 4 Sep 2014

Louise Karlskov Skyggebjerg (Speaker)

Department of Physics

**Description**

Indlæg: Making the history of industrial work (relevant for tomorrow's public)

**Related event**

Worklab Conference

03/09/2014 → 06/09/2014

Steyr, Austria

Activity: Talks and presentations › Conference presentations

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**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.

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**9th International Workshop on Strong Microwaves and Terahertz Waves**

Period: 26 Jul 2014

Stefan Kragh Nielsen (Participant)

Department of Physics

Plasma Physics and Fusion Energy

**Related event**
Three-Dimensional X-ray Diffraction (3DXRD) microscopy for studying dynamics in polycrystalline materials
Period: 15 Jul 2014
Jette Oddershede (Lecturer)
Department of Physics
Neutrons and X-rays for Materials Physics

Description
Seminar at Department of Materials, University of Oxford, UK

Related external organisation
Unknown external organisation
Activity: Talks and presentations › Conference presentations

51st Culham Plasma Physics Summer School
Magnus Dam (Participant)
Department of Applied Mathematics and Computer Science
Mathematics
Department of Physics
Plasma Physics and Fusion Energy

Description
Presented a poster.
Documents:
LH transition poster by M Dam (2014)

Related event
51st Culham Plasma Physics Summer School
14/07/2014 → 25/07/2014
Abingdon, Oxfordshire, United Kingdom
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Chair of the Council of the European XFEL (External organisation)
Period: 1 Jul 2014 → 30 Jun 2018
Martin Meedom Nielsen (Chairman)
Department of Physics
Neutrons and X-rays for Materials Physics

Description
The Council is the shareholders representation and, the supreme organ of the European XFEL.EU
Chair of the European XFEL Council, the supreme organ of the European XFEL.

Body type: Governing body
Degree of recognition: International

Related external organisation
Chair of the Council of the European XFEL
Activity: Membership › Membership of committees, commissions, boards, councils, associations, organisations, or similar
Deformation-induced intragranular orientation spread in ferrite investigated by 3DXRD and forward modeling
Period: 1 Jul 2014
Jette Oddershede (Lecturer)
Department of Physics
Neutrons and X-rays for Materials Physics

Related event
2nd International Congress on 3D Materials Science
29/06/2014 → 02/07/2014
Annecy, France
Activity: Talks and presentations › Conference presentations

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

Adding the Environmental TEM to the In Situ Toolbox for Catalyst Characterization
Period: 16 Jun 2014
Christian Danvad Damsgaard (Invited speaker)
Center for Electron Nanoscopy
DTU Danchip
Department of Physics
Experimental Surface and Nanomaterials Physics

Description
Nordic keynote presenter

Related external organisation
Unknown external organisation
Activity: Talks and presentations › Conference presentations

A comparative study of Pd2Ga catalyst
Period: 15 Jun 2014
Elisabetta Maria Fiordaliso (Keynote speaker)
Center for Electron Nanoscopy
DTU Danchip
Department of Physics
**Description**
Keynote lecture at the EDPIC 14 conference.

**Related event**

**European Powder Diffraction Conference 2014**
18/06/2014 → 18/06/2014
Århus, Denmark

Activity: Talks and presentations › Conference presentations

**Universeum Network Meeting**
Period: 13 Jun 2014
Laila Zwisler (Speaker)
Department of Physics

**Description**
Three in One - Heritage, Research and Dissimation at The Technical University of Denmark.

Links:
http://universeum.it/meetings.html (Link to Universeum events)

**Related event**

**Universeum Network Meeting: Enhancing University Heritage-Based Research**
11/06/2014 → 14/06/2014
Hamburg, Germany

Activity: Talks and presentations › Conference presentations

**STAC (Scientific and Technical Advisory Committee) EUROfusion (External organisation)**
Period: 1 Jun 2014 → 31 May 2018
Jens Juul Rasmussen (Participant)
Department of Physics
Plasma Physics and Fusion Energy

**Description**
Advisory board for the EUROfusion consortium.
Workplan, Workprogramme, Assessments, Evaluation

Body type: Committee
Degree of recognition: International

**Related external organisation**

**STAC (Scientific and Technical Advisory Committee) EUROfusion**
Activity: Membership › Membership of committees, commissions, boards, councils, associations, organisations, or similar

**Wave-Flow Interaction in Geophysics, Climate, Astrophysics, and Plasmas**
Period: 1 Jun 2014 → 21 Jun 2014
Jens Juul Rasmussen (Participant)
Department of Physics
Plasma Physics and Fusion Energy

**Description**
Participation in the KITP-programme on

Kavli Institute for Theoretical Physics (KITP), University of California
Documents:
KITP_activity report -2014
Links:
Related event

Wave-Flow Interaction in Geophysics, Climate, Astrophysics, and Plasmas
24/03/2014 → 21/06/2014
Santa Barbara, CA, United States
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Ready for China? Scandinavian Businesses in China 1890-2014
Period: 27 May 2014
Louise Karlskov Skyggebjerg (Speaker)
Department of Physics
Description
Sammen med Kristoffer Jensen indlægget "A piece of Denmark? - Danish manufacturing in China today"

Related event

Ready for China? Scandinavian Businesses in China 1890-2014
27/05/2014 → 28/05/2014
København, Denmark
Activity: Other

EUROfusion IPH Code Development (CD) Project Board (External organisation)
Period: 1 Apr 2014 → 1 Apr 2018
Jens Juul Rasmussen (Participant)
Department of Physics
Plasma Physics and Fusion Energy
Description
Project board with 28 members
Degree of recognition: International

Related external organisation

EUROfusion IPH Code Development (CD) Project Board
Activity: Membership › Membership of committees, commissions, boards, councils, associations, organisations, or similar

New Waves. Emergent perspectives in Nordic history of industrialization and innovation
Period: 24 Mar 2014
Louise Karlskov Skyggebjerg (Invited speaker)
Department of Physics
Description
Indlæg: The non spectacular on display - everyday life at work and at home

Related event

New Waves. Emergent perspectives in Nordic history of industrialization and innovation: A monthly symposia series arranged by Aalto University, University of Helsinki and Finnish Economic History Association
17/02/2014 → 28/04/2014
Helsinki, Finland
Activity: Talks and presentations › Conference presentations

Investigations of plasma turbulence
Period: 18 Mar 2014
Anders Henry Nielsen (Lecturer)
Department of Physics
Related event

**[Fluid-DTU] Fluid*DTU seminar**
18/03/2014 → …
Lyngby, Denmark
Activity: Talks and presentations › Conference presentations

**Fusionsenergi: Atomenergi i det 21. århundrede**
Period: 12 Mar 2014 → 9 Apr 2014
Jens Juul Rasmussen (Lecturer)
Department of Physics
Plasma Physics and Fusion Energy

**Description**
2 Lectures ved Folkeuniversitetet i København Foråret 2014
2 forlæsninger om Fusionsenergi i en forelæsningsrække på 5 forelæsninger om Atomenergi i det 21. århundrede (B. Lohmann Andersen og Jens Juul Rasmussen)

**Related external organisation**

**Unknown external organisation**
Activity: Talks and presentations › Conference presentations

**Inverse scattering: from formulation to application**
Period: 10 Mar 2014
Mirza Karamehmedovic (Invited speaker)
Department of Applied Mathematics and Computer Science
Scientific Computing
Department of Physics
Neutrons and X-rays for Materials Physics

**Related event**

**Lecture at International University of Sarajevo**
10/03/2014 → …
Sarajevo, Bosnia and Herzegovina
Activity: Talks and presentations › Conference presentations

**Strain Mechanisms in Polycrystalline BaTiO3 Measured at the Single Grain Level during In-Situ Electrical Poling**
Period: 19 Feb 2014
Jette Oddershede (Lecturer)
Department of Physics
Neutrons and X-rays for Materials Physics

**Description**
Invited presentation

**Related event**

**TMS 2014 143rd Annual Meeting and Exhibition**
18/02/2014 → 20/02/2014
San Diego, CA, United States
Activity: Talks and presentations › Conference presentations
Hydrodynamics of Choanoflagellate Feeding
Period: 24 Nov 2013
Anders Peter Andersen (Lecturer)
Department of Physics
Biophysics and Fluids
Links:
http://meetings.aps.org/Meeting/DFD13/Session/D18.5

Related external organisation
Unknown external organisation
Activity: Talks and presentations › Conference presentations

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.

Temperature fluctuation measurements – Energy flux – Power deposition
Period: 4 Nov 2013 → 8 Nov 2013
Jens Juul Rasmussen (Lecturer)
Department of Physics
Plasma Physics and Fusion Energy

Description
Lecture at: Workshop on 3D SOL modelling; DTU Physics; DTU Rise Campus, Roskilde, Denmark, 04 – 08 November 2013

Related event
Workshop on 3D SOL modelling
04/11/2013 → 08/11/2013
Roskilde, Denmark
Activity: Talks and presentations › Conference presentations

Phonons in the presence of current: Exciting atomic motion
Period: 31 Oct 2013
Mads Brandbyge (Invited speaker)
Department of Micro- and Nanotechnology
Theoretical Nanoelectronics
Department of Physics

Description
Invited talk at 543 WE-Heraeus-Seminar, Physikzentrum Bad Honnef, Germany.
Three-Dimensional X-ray Diffraction (3DXRD) microscopy for studying dynamics in polycrystalline materials
Period: 25 Oct 2013
Jette Oddershede (Lecturer)
Department of Physics
Neutrons and X-rays for Materials Physics

Description
CLASSE seminar at the Cornell High Energy Synchrotron Source, CHESS, Cornell University, Ithaca NY, USA

Related external organisation
Unknown external organisation
Activity: Talks and presentations › Conference presentations

De nordiske velfærdssamfunds immaterielle kulturav
Period: 24 Oct 2013
Louise Karlskov Skyggebjerg (Organizer)
Department of Physics

Related event
De nordiske velfærdssamfunds immaterielle kulturav
24/10/2013 → 24/10/2013
København, Denmark
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Dansk Teknologihistorisk Selskabs Årsmøde
Period: 14 Sep 2013
Laila Zwisler (Organizer)
Department of Physics
Office for Study Programmes and Student Affairs
Department of Mechanical Engineering
Links:
http://www.teknologihistorie.dk/

Related event
Dansk Teknologihistorisk Selskabs Årsmøde: Den danske ingeniørs historiske konstruktion
14/09/2013 → 14/09/2013
Kgs. Lyngby, Denmark
Activity: Attending an event › Participating in or organising a conference

Strain Mechanisms in Polycrystalline BaTiO3 Measured at the Single Grain Level during In-Situ Electrical Poling
Period: 11 Sep 2013
Jette Oddershede (Lecturer)
Department of Physics
Neutrons and X-rays for Materials Physics

Related event
7th International Conference on Mechanical Stress Evaluation by Neutron and Synchrotron Radiation  
10/09/2013 → 12/09/2013  
Sydney, Australia  
Activity: Talks and presentations › Conference presentations

4th Sino-Danish Autumn School on Fusion Plasma Physics and Technology  
Period: 10 Sep 2013  
Jens Juul Rasmussen (Guest lecturer)  
Department of Physics  
Plasma Physics and Fusion Energy  
Description  
Impurity transport, particle pinch, and density peaking in toroidal magnetized plasma.

Related event

4th Sino-Danish Autumn School on Fusion Plasma Physics and Technology  
Period: 9 Sep 2013 → 12 Sep 2013  
Anders Henry Nielsen (Organizer)  
Department of Physics  
Plasma Physics and Fusion Energy  
Description  
Organizer from the Danish side.

Related event

4th Sino-Danish Autumn School on Fusion Plasma Physics and Technology  
Period: 9 Sep 2013 → 12 Sep 2013  
Volker Naulin (Organizer)  
Department of Physics  
Plasma Physics and Fusion Energy  
Description
Organizer from the Danish side

**Related event**

**4th Sino-Danish Autumn School on Fusion Plasma Physics and Technology**
09/09/2013 → 12/09/2013  
Dalian, China  
Activity: Attending an event › Participating in or organising a conference

**Description**
Lecture: “Particle transport in toroidal magnetized plasma”.

**Related event**

**4th Sino-Danish Autumn School on Fusion Plasma Physics and Technology**
Period: 9 Sep 2013  
Jens Juul Rasmussen (Guest lecturer)  
Department of Physics  
Plasma Physics and Fusion Energy

**Related event**

**4th Sino-Danish Autumn School on Fusion Plasma Physics and Technology**
Period: 9 Sep 2013  
Volker Naulin (Guest lecturer)  
Department of Physics  
Plasma Physics and Fusion Energy

**Related event**

**4th Sino-Danish Autumn School on Fusion Plasma Physics and Technology**
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**

**Functional dependent errors in DFT calculations for Li-air batteries**
Period: 9 Sep 2013  
Rune Christensen (Speaker)

**Related event**

**2nd ReLiable Li-Air Workshop**
09/09/2013 → 10/09/2013  
Copenhagen, Denmark  
Activity: Talks and presentations › Conference presentations
Particle transport in toroidal magnetized plasma
Period: 9 Sep 2013
Jens Juul Rasmussen (Lecturer)
Department of Physics
Plasma Physics and Fusion Energy

Description
Lecture 09-09-2013

Related event
4th Sino-Danish Autumn School on Fusion Plasma Physics and Technology
09/09/2013 → 12/09/2013
Dalian, China
Activity: Talks and presentations › Conference presentations

11th European Congress on Catalysis
Period: 1 Sep 2013 → 6 Sep 2013
Elisabetta Maria Fiordaliso (Participant)
Center for Electron Nanoscopy
Department of Physics

Description
Poster contribution.

Poster contribution.

Related event
11th European Congress on Catalysis
01/09/2013 → 06/09/2013
Lyon, France
Activity: Attending an event › Participating in or organising a conference

24th International Congress of History of Science, Technology and Medicine
Period: 24 Jul 2013
Laila Zwisler (Speaker)
Department of Physics

Description
University-Industry Transfer

Related event
24th International Congress of History of Science, Technology and Medicine: Knowledge at Work
21/07/2013 → 27/07/2013
Manchester, United Kingdom
Activity: Talks and presentations › Conference presentations

Culham Centre for Fusion Energy
Period: 10 Jun 2013 → 23 Aug 2013
Morten Stejner Pedersen (Visiting researcher)
Department of Physics
Plasma Physics and Fusion Energy

Description
Responsible Officer for HRTS data analysis on JET

In 2013 Morten Stejner Pedersen was on secondment at JET from May 7 to May 17 and again during C31 from June 10 to August 23. At JET he worked with the electron kinetics group fulfilling the role of Responsible Officer for data analysis on
the High Resolution Thomson Scattering (HRTS) diagnostic system. As such he was responsible for maintenance of the HRTS data analysis codes, for updating and implementing new calibrations for HRTS in C31 and for validation of HRTS data.

Activity: Visiting an external institution › Visiting another research institution

**Scandem 2013 - Annual Meeting of the Nordic Microscopy Society**

*Period: 10 Jun 2013 → 14 Jun 2013*

*Elisabetta Maria Fiordaliso (Participant)*

Center for Electron Nanoscopy

Department of Physics

**Description**

Oral presentation.

Conference.

**Related event**

**Scandem 2013 - Annual Meeting of the Nordic Microscopy Society**

10/06/2013 → 14/06/2013

Copenhagen, Denmark

Activity: Attending an event › Participating in or organising a conference

**Light Scattering**

*Period: 27 May 2013 → 28 May 2013*

*Mirza Karamehmedovic (Participant)*

Department of Applied Mathematics and Computer Science

Scientific Computing

Department of Physics

**Description**

1) Karamehmedović, M., A sparse numerical model for optical characterisation of nanoparticles on rough surfaces
2) Thomas, S., Matyssek, C., Hergert, W., Kiewidt, L., Karamehmedović, M., and Wriedt, T., Optimization of plasmonic nanostructures excited by light or electron beams: A Generalized Multiparticle Mie Solution study

**Related event**

**Light Scattering: Simulation and Inversion**

27/05/2013 → 28/05/2013

Bremen, Germany

Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

**Self-organization and generation of large scale flows in quasi 2D turbulence**

*Period: 7 May 2013*

*Jens Juul Rasmussen (Speaker)*

Department of Physics

Plasma Physics and Fusion Energy

**Description**

**Related event**

**Fluid*DTU Seminar**

07/05/2013 → ...

Kgs. Lyngby, Denmark

Activity: Talks and presentations › Conference presentations
Electron-phonon coupling and molecular dynamics in the presence of current
Period: 1 May 2013
Mads Brandbyge (Lecturer)
Department of Physics
Department of Micro- and Nanotechnology
Theoretical Nanoelectronics

Description
Invited talk at "Workshop on Controlled Atomic Dynamics on Solid Surfaces: Atom and Molecular Manipulation (UEBA13)", San Sebastian, Spain.

Related event
Workshop on Controlled Atomic Dynamics on Solid Surfaces: Atom and Molecular Manipulation
13/05/2013 → 16/05/2013
San Sebastián, Spain
Activity: Talks and presentations › Conference presentations

Status of CTS data analysis
Period: 13 Apr 2013
Morten Stejner Pedersen (Speaker)
Department of Physics
Plasma Physics and Fusion Energy

Description
Seminar at IPP-Garching on CTS data analysis. Presented first bulk-ion measurements by CTS at AUG including a comparison of CTS and CXRS results for ion temperature and plasma rotation.

Related external organisation
Unknown external organisation
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

Internationalt formidlingsseminar
Period: 12 Mar 2013 → 14 Mar 2013
Laila Zwisler (Participant)
Department of Physics

Related event
Internationalt formidlingsseminar: Museer på tværs
12/03/2013 → 14/03/2013
Electron-phonon coupling and molecular dynamics in the presence of current
Period: 7 Mar 2013
Mads Brandbyge (Lecturer)
Department of Physics
Department of Micro- and Nanotechnology
Theoretical Nanoelectronics

Description
Invited talk at CECAM workshop "Molecular electronics: Quo vadis??, Bremen, Germany.
Links:
http://www.cecam.org/workshop-4-801.html?presentation_id=8754

Related event
CECAM Workshop Molecular electronics: Quo vadis?
04/03/2013 → 08/03/2013
Bremen, Germany
Activity: Talks and presentations › Conference presentations

Plasma turbulence and transport
Period: 13 Dec 2012
Jens Juul Rasmussen (Lecturer)
Department of Physics
Plasma Physics and Fusion Energy

Description
Lecture at EURATOM-DTU Association Day
DTU Risø Campus
4000 Roskilde

Related event
EURATOM-DTU Association Day
13/12/2012 → …
Roskilde, Denmark
Activity: Talks and presentations › Conference presentations

HDR defense for David Fabre, IMFT, Toulouse (External organisation)
Period: 12 Dec 2012
Tomas Bohr (Participant)
Department of Physics
Biophysics and Fluids
Degree of recognition: International

Related external organisation
HDR defense for David Fabre, IMFT, Toulouse
Activity: Membership › Membership of commitees, commissions, boards, councils, associations, organisations, or similar

Computational Screening of Mixed Metal Halide Ammines
Period: 4 Dec 2012
Peter Bjørre Jensen (Lecturer)
Department of Energy Conversion and Storage
Vedvarende energi: Fusionsenergi
Period: 14 Nov 2012
Jens Juul Rasmussen (Lecturer)
Department of Physics
Plasma Physics and Fusion Energy
Description
Forelæsning ved Folkeuniversitetet AU, Herning, 14.-11.-2012
Related external organisation
Unknown external organisation
Activity: Talks and presentations › Conference presentations

Fusionsenergi – hvordan går det med at efterligne solen?
Period: 13 Nov 2012
Søren Bang Korsholm (Lecturer)
Department of Physics
Plasma Physics and Fusion Energy
Description
Videnskabsfolk har siden 50'erne arbejdet intensivt på at realisere fusionsenergi som en reel energikilde på jorden. Fusionsenergi er solens og stjernernes energiform, og drømmen er at efterligne solen i kraftværker på jorden. Lykkes det vil menneskeheden have en energikilde med uudtømmelige energiressourcer, der vil frigøre os af afhængighed af fossile brændsler.
Links:
http://aalborg.unf.dk/
http://aalborg.unf.dk/program.php?id=1008477&arr=Fusionsenergi+%3F+hvordan+g%E5r+med+at+et%3F
Plasmaturbulens og -transport
Period: 6 Nov 2012
Jens Juul Rasmussen (Lecturer)
Department of Physics
Plasma Physics and Fusion Energy

Description
Lecture at
Fusionsklassen Scientalentør
Mærsk Mc-Kinney Møller Videncenter Sorø

Related external organisation
Unknown external organisation
Activity: Talks and presentations › Conference presentations

MUFLOW12-Colloquium: Spontaneous symmetry breaking on fluid surfaces
Period: 29 Oct 2012
Tomas Bohr (Invited speaker)
Department of Physics
Biophysics and Fluids

Related event
Multiscale Complex Fluid Flows and Interfacial Phenomena
29/10/2012 → 01/11/2012
Dresden, Germany
Activity: Talks and presentations › Conference presentations

Bæredygtig energi skal redde fremtidens klima: Fusionsenergi
Period: 23 Oct 2012
Jens Juul Rasmussen (Lecturer)
Department of Physics
Plasma Physics and Fusion Energy

Description
Forelæsning ved Folkeuniversitetet KU
23. Oktober 2012

Related external organisation
Unknown external organisation
Activity: Talks and presentations › Conference presentations

SEM 2012: Scanning Electron Microscopy
Elisabetta Maria Fiordaliso (Participant)
Center for Electron Nanoscopy
Department of Physics

Description
SEM course.

Related event
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

Development and characterization of novel catalysts for methanol synthesis from CO2 and hydrogen
Period: 10 Oct 2012
Christian Danvad Damsgaard (Invited speaker)
Center for Electron Nanoscopy
Department of Physics
Experimental Surface and Nanomaterials Physics
Documents:
PDF
Links:
http://www.bccms.uni-bremen.de/veranstaltungen/2012/cecam_co2/

Related event
Future challenges in CO2 reduction - International CECAM-Workshop
08/10/2005 → 12/10/2012
Bremen, Germany
Activity: Talks and presentations › Conference presentations

Local stress distributions studied at the single grain level
Period: 9 Oct 2012
Jette Oddershede (Lecturer)
Department of Physics
Neutrons and X-rays for Materials Physics

Related event
9th Conference on Residual Stress
07/10/2012 → 10/10/2012
Garmisch-Partenkirschen, Germany
Activity: Talks and presentations › Conference presentations

Structures and nonlocality in magnetically confined plasmas
Period: 8 Oct 2012
Volker Naulin (Invited speaker)
Department of Physics
Plasma Physics and Fusion Energy

Related event

17th Fall Seminar on Nonlinear Dynamics
Period: 07/10/2012 → 10/10/2012
Bayreuth, Germany
Activity: Talks and presentations › Conference presentations

Teknologi måler utilfredshed og velvære
Laila Zwisler (Other)
Department of Physics

Description
Udstilling på DTU Bibliotek

Udarbejdet af Teknologihistorie DTU og DTU Bibliotek.
Organizer.
Activity: Other

ETEM investigation of new catalysts for methanol synthesis
Period: 27 Sep 2012
Christian Danvad Damsgaard (Invited speaker)
Center for Electron Nanoscopy
Department of Physics
Experimental Surface and Nanomaterials Physics

Description
Invited speaker at Karlsruher Institute of Technology, Host: Professor Jan-Dierk Grunwaldt

Related external organisation

Unknown external organisation
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
Period: 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

Dansk Teknologihistorisk Selskab (External organisation)
Period: 20 Sep 2012
Laila Zwisler (Secretary)

Description
Selskabet har til formål at fremme teknologihistorisk forskning, undervisning og formidling i Danmark. Selskabet virker for udveksling af viden mellem enkeltpersoner og institutioner, der arbejder med teknologihistoriske emner.

Body type: Selskab

Related external organisation

Dansk Teknologihistorisk Selskab
Activity: Membership › Board duties in companies, associations, or public organisations

Pressure driven instabilities in magnetized plasmas: The interchange instability
Period: 18 Sep 2012
Jens Juul Rasmussen (Invited speaker)

Department of Physics
Plasma Physics and Fusion Energy

Related event

3rd Sino Danish Autumn School on Fusion Plasma Physics and Technology: SDC Autumn School Plasma Physics
17/09/2012 → 20/09/2012
Hefei, China
Activity: Talks and presentations › Conference presentations

3rd Sino Danish Autumn School on Fusion Plasma Physics and Technology
Period: 17 Sep 2012 → 20 Sep 2012
Jens Juul Rasmussen (Guest lecturer)

Department of Physics
Plasma Physics and Fusion Energy

Description
Topic: Pressure driven instabilities in magnetized plasmas: The interchange instability

3rd Sino Danish Autumn School on Fusion Plasma Physics and Technology
17-20 September 2012
Institute of Plasma Physics, Chinese Academy of Sciences
Hefei, China
Related event

3rd Sino Danish Autumn School on Fusion Plasma Physics and Technology: SDC Autumn School Plasma Physics
17/09/2012 → 20/09/2012
Hefei, China
Activity: Talks and presentations › Guest lectures, external teaching and course activities at other universities

3rd Sino Danish Autumn School on Fusion Plasma Physics and Technology
Period: 17 Sep 2012 → 20 Sep 2012
Jens Juul Rasmussen (Guest lecturer)
Department of Physics
Plasma Physics and Fusion Energy

Description
Topic: Turbulent particle transport in magnetized plasma

3rd Sino Danish Autumn School on Fusion Plasma Physics and Technology
SDC - Sino Danois Center for Education and Research
Institute of Plasma Physics, Chinese Academy of Sciences
Hefei, China

Related event

Turbulent particle transport in magnetized plasma
Period: 17 Sep 2012
Jens Juul Rasmussen (Invited speaker)
Department of Physics
Plasma Physics and Fusion Energy

Description
SDC - Sino Danois Center for Education and Research

Related event

Rådgivningsgruppen for Fusionsenergi (External organisation)
Period: 1 Sep 2012 → 1 Jan 2016
Volker Naulin (Participant)
Department of Physics
Plasma Physics and Fusion Energy

Related external organisation

Rådgivningsgruppen for Fusionsenergi
Activity: Membership › Membership of committees, commissions, boards, councils, associations, organisations, or similar

Transport properties and atomic dynamics of nanoconductors from first principles calculations
Period: 1 Sep 2012
Mads Brandbyge (Lecturer)
Department of Physics
Department of Micro- and Nanotechnology
Theoretical Nanoelectronics

**Description**
Invited talk at IUMRS-Int. Conf. on Elec. Materials (IUMRS-ICEM 2012), Yokohama, Japan.

**Related external organisation**
Unknown external organisation
Activity: Talks and presentations › Conference presentations

**In situ investigation of catalysts for alcohol synthesis**
Period: 15 Jun 2012
Christian Danvad Damsgaard (Speaker)
Center for Electron Nanoscopy
Department of Physics
Experimental Surface and Nanomaterials Physics
Documents:
Scandem_final.pdf
Links:
http://sites.web123.no/AtlanticReiser/uib/Scandem2012/home.cfm

**Related event**
**Scandem 2012 - Annual Meeting of the Nordic Microscopy Society**
12/06/2012 → 15/06/2012
Bergen, Norway
Activity: Talks and presentations › Conference presentations

**XIII Universum Network Meeting**
Period: 15 Jun 2012
Laila Zwisler (Speaker)
Department of Physics

**Description**
Gave paper written by Maria Lanng and Laila Zwisler
Gave paper "Different Approaches to Cultural Heritage"

**Related event**
**XIII Universum Network Meeting**
14/06/2012 → 16/06/2012
Trondheim, Norway
Activity: Talks and presentations › Conference presentations

**ETEM study of deactivation of NiGa nanoparticles as catalyst for methanol synthesis**
Period: 11 Jun 2012
Christian Danvad Damsgaard (Speaker)
Center for Electron Nanoscopy
Department of Physics
Experimental Surface and Nanomaterials Physics
Documents:
ETEM study of deactivation of NiGa nanoparticles as catalyst for methanol synthesis
Related event

15th Nordic Symposium on Catalysis
10/06/2012 → 12/06/2012
Mariehamn, Åland Islands
Activity: Talks and presentations › Conference presentations

Turbulence and Transport in Magnetically Confined Plasma
Period: 4 Jun 2012 → 8 Jun 2012
Jens Juul Rasmussen (Invited speaker)
Department of Physics
Plasma Physics and Fusion Energy

Description
Member of International programme committee

Related event

6th International Conference on Solitons, Collapses and Turbulence: Achievements, Developments and Perspectives
04/06/2012 → 08/06/2012
Akademgorodok, Novosibirsk, Russian Federation
Activity: Talks and presentations › Conference presentations

Interview til Apropos på DR
Period: 8 May 2012
Laila Zwisler (Participant)
Department of Physics

Description
Interview til Apropos på DR

Related external organisation

Danmarks Radio
Denmark
Activity: Other

Temporally resolved plasma composition measurements by collective Thomson scattering in TEXTOR
Period: 6 May 2012
Morten Stejner Pedersen (Invited speaker)
Department of Physics
Plasma Physics and Fusion Energy

Related event

19th Topical Conference High-Temperature Plasma Diagnostics
06/05/2012 → 12/05/2012
Monterey, California, United States
Activity: Talks and presentations › Conference presentations

Theory and first principles calculations of current-induced atomic dynamics
Period: 1 May 2012
Mads Brandbyge (Lecturer)
Department of Physics
Department of Micro- and Nanotechnology
Theoretical Nanoelectronics
Description
Invited talk at the "Int. Workshop on Computational Electronics (IWCE) 2012", Madison, Wisconsin, USA.

Related external organisation

Unknown external organisation
Activity: Talks and presentations › Conference presentations

Inverse Problems and Numerical Methods in Applications
Period: 8 Mar 2012 → 9 Mar 2012
Mirza Karamahmedovic (Organizer)
Department of Applied Mathematics and Computer Science
Scientific Computing
Department of Physics
Documents:
Book_of_Abstracts

Related event

Inverse Problems and Numerical Methods in Applications
08/03/2012 → 09/03/2012
Bremen, Germany
Activity: Attending an event › Participating in or organising a conference

Fast Acquisition of Thomson Scattering for Fusion Plasma Composition Measurements
Period: 5 Mar 2012
Morten Stejner Pedersen (Invited speaker)
Department of Physics
Plasma Physics and Fusion Energy

Related event

5th Annual Pan-European Science & Big Physics Symposium
05/03/2012 → 05/03/2012
Zurich, Switzerland
Activity: Talks and presentations › Conference presentations

Electronic transport, Joule-heating, and current-driven atomic dynamics in molecular contacts – theory and simulations
Period: 1 Mar 2012
Mads Brandbyge (Lecturer)
Department of Physics
Department of Micro- and Nanotechnology
Theoretical Nanoelectronics

Description
Invited talk at the Deutschen Physikalischen Gesellschaft (DPG), spring meeting, 2012.

Related external organisation

Unknown external organisation
Activity: Talks and presentations › Conference presentations

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.

Dobbeltforelæsning om Fusionsenergi i kurset for "Vedvarende Energi"
Period: 30 Jan 2012
Jens Juul Rasmussen (Lecturer)
Department of Physics
Plasma Physics and Fusion Energy

Description
Folkeuniversitetet, Emdrup Campus, Aarhus Universitet

Dobbeltforelæsning om Fusionsenergi i kurset for "Vedvarende Energi“ Folkeuniversitetet i Emdrup, Aarhus Universitet.

Related event

Vedvarende Energi: Fusionsenergi
30/01/2012 → …
Emdrup, København NV, Denmark
Activity: Talks and presentations › Guest lectures, external teaching and course activities at other universities

Culham Centre for Fusion Energy
Period: 16 Jan 2012 → 10 Feb 2012
Morten Stejner Pedersen (Visiting researcher)
Department of Physics

Description
Secondment to Joint European Torus (JET), located at Culham Centre for Fusion Energy (CCFE): Working with the JET electron kinetics group

In 2011 Morten Stejner was on secondment at JET during C29 from January 16 to February 10. At JET he participated in work within the electron kinetics group to validate data from electron temperature diagnostics based on incoherent Thomson scattering measurements and electron cyclotron emission spectroscopy (the KE3, KE11, KK1 and KK3 diagnostics). Measurements with these diagnostics had previously shown discrepancies between the inferred electron temperatures, and the origin of these discrepancies was investigated based on both historical data and more recent data from C28 and C29 incorporating updated calibrations for both types of diagnostics. This work was continued from another secondment period in late 2011.

Activity: Visiting an external institution › Visiting another research institution

Measuring Grain Resolved Stresses during in situ Plastic Deformation using 3DXRD
Period: 6 Jan 2012
Jette Oddershede (Lecturer)
Department of Physics
Neutrons and X-rays for Materials Physics

Description
Invited presentation
Documents:
Oddershede_3page_revised

Related event
Plants as dynamical systems: Universality and optimality of osmotically driven sap-flow
Period: 4 Jan 2012
Tomas Bohr (Invited speaker)
Department of Physics
Biophysics and Fluids

Related event

Dynamics Days 2012
04/01/2012 → 07/01/2012
Baltimore, MD, United States
Activity: Talks and presentations › Conference presentations

Plants as dynamical systems: Universality and optimality of osmotically driven sap-flow
Period: 4 Jan 2012
Tomas Bohr (Invited speaker)
Department of Physics
Biophysics and Fluids

Related event

Dynamics Days 2012
04/01/2012 → 07/01/2012
Baltimore, MD, United States
Activity: Talks and presentations › Conference presentations

EFDA . Steering Committee (External organisation)
Period: 1 Jan 2012 → 1 Jan 2014
Volker Naulin (Participant)
Department of Physics
Plasma Physics and Fusion Energy

Description
EFDA - European Fusion Development Association
Degree of recognition: International

Related external organisation

EFDA . Steering Committee
Activity: Membership › Membership of committees, commissions, boards, councils, associations, organisations, or similar

EFDA . Topical Group Transport (External organisation)
Period: 1 Jan 2012 → 1 Jan 2014
Volker Naulin (Participant)
Department of Physics
Plasma Physics and Fusion Energy

Description
EFDA - European Fusion Development Association
Degree of recognition: International

Related external organisation
EFDA. Topical Group Transport
Activity: Membership › Membership of committees, commissions, boards, councils, associations, organisations, or similar

**Fusion 4 Energy (External organisation)**
Period: 1 Jan 2012 → 1 Jan 2014
Volker Naulin (Participant)

Department of Physics
Plasma Physics and Fusion Energy

**Description**
Fusion 4 Energy (F4E) is the European Union’s Joint Undertaking for ITER and the Development of Fusion Energy. The organisation was created under the Euratom Treaty by a decision of the Council of the European Union
Degree of recognition: International

**Related external organisation**

**Fusion 4 Energy**
Activity: Membership › Membership of committees, commissions, boards, councils, associations, organisations, or similar

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**Det Faglige Råd for Nyere Tids Kulturhistorie (External organisation)**
Period: 2011 → 2013
Louise Karlskov Skyggebjerg (Participant)

Department of Physics

**Description**
Rådgivende organ for Kulturavstyrelsen
Valgt medlem

**Related external organisation**

**Det Faglige Råd for Nyere Tids Kulturhistorie**
Activity: Membership › Membership of committees, commissions, boards, councils, associations, organisations, or similar

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**Styrelsen for Forskning og Innovation (External organisation)**
Period: 17 Aug 2011 → 1 Apr 2014
Søren Bang Korsholm (Participant)

Department of Physics
Plasma Physics and Fusion Energy

**Description**
Industrial Liaison Officer Network to the European Southern Observatory

The ESO ILO Network is the link between ESO and the industry of the member states. The ILOs assist ESO and the industry in preparation for tender actions.

As the Danish Industrial Liaison Officer (ILO) to the European Southern Observatory (ESO) the role is to be the link between ESO and Danish industry in preparation for tender actions from ESO. The ILO is part of the ESO ILO Network and participate in the ILO meetings and other ESO events. The ILO's are nominated by the national member state Council/finance committee representatives.

Body type: International organisation
Degree of recognition: International
Links:
http://www.eso.org/public/industry/cp/ILO/ILO_Contact_Details_for_web.pdf (List of ESO ILOs)

**Related external organisation**

**Styrelsen for Forskning og Innovation**
Denmark
**Euspen Challenge**
Period: Jul 2011 → ...
Elisabetta Maria Fiordaliso (Participant)
Department of Physics
Center for Electron Nanoscopy

**Description**
Challenge for PhD students.

**Related event**

**Euspen Challenge**
20/07/2011 → ...
Cambridge, United Kingdom
Activity: Attending an event › Participating in or organising a conference

**Microreactors for heterogenous catalysis: Oral presentation at Nordic Semiconductor Meeting 2011**
Period: 19 Jun 2011
Jakob Lind Olsen (Speaker)
Department of Physics

**Description**
Place: Aarhus, Denmark
Documents:
prod11327574822908.NSM2011[1].pdf

**Related external organisation**

**Unknown external organisation**
Activity: Talks and presentations › Conference presentations

**Microreactors for heterogenous catalysis: Oral presentation at Nordic Semiconductor Meeting 2011**
Period: 19 Jun 2011
Peter Christian Kjærgaard Vesborg (Speaker)
Department of Physics
Experimental Surface and Nanomaterials Physics

**Description**
Place: Aarhus, Denmark
Documents:
prod11327574822908.NSM2011[1].pdf

**Related external organisation**

**Unknown external organisation**
Activity: Talks and presentations › Conference presentations

**Microreactors for heterogenous catalysis: Oral presentation at Nordic Semiconductor Meeting 2011**
Period: 19 Jun 2011
Ib Chorkendorff (Speaker)
Department of Physics
Experimental Surface and Nanomaterials Physics
**Description**  
Place: Aarhus, Denmark  
Documents:  
prod11327574822908.NSM2011[1].pdf

**Related external organisation**

**Unknown external organisation**  
Activity: Talks and presentations › Conference presentations

**European XFEL (External organisation)**  
Period: 1 Jun 2011 → 30 Jun 2014  
Martin Meedom Nielsen (Participant)  
Department of Physics  
Neutrons and X-rays for Materials Physics

**Description**  
Delegate to the Council of the European XFEL, appointed by DASTI

Delegate to the Council of the European XFEL, appointed by DASTI

**Body type:** Governing Body  
**Degree of recognition:** International

**Related external organisation**

**European XFEL**  
Germany  
Activity: Membership › Membership of committees, commissions, boards, councils, associations, organisations, or similar

**Nano Structures on Surfaces and Light Scattering**  
Mirza Karamehmedovic (Participant)  
Department of Applied Mathematics and Computer Science  
Scientific Computing  
Department of Physics

**Description**  
M. Karamehmedović and T. Wriedt. Sizing of highly conductive nanowires on substrates

**Related event**

**Nano Structures on Surfaces and Light Scattering**  
24/03/2011 → 25/03/2011  
Bremen, Germany  
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

**Society for the History of Technology**  
Period: Oct 2010  
Louise Karlskov Skyggebjerg (Speaker)  
Department of Physics

**Related event**

**Society for the History of Technology: Annual Meeting 2010**  
30/09/2010 → 03/10/2010  
Tacoma, United States  
Activity: Talks and presentations › Conference presentations
Congresso nazionale di catalisi
Period: 19 Sep 2010
Elisabetta Maria Fiordaliso (Participant)
Department of Physics
Center for Electron Nanoscopy

Description
Oral contribution.
Conference.

Related event
Congresso nazionale di catalisi
19/09/2010 → …
Palermo, Italy
Activity: Attending an event › Participating in or organising a conference

Idecat conference
Period: 12 May 2010
Elisabetta Maria Fiordaliso (Participant)
Department of Physics
Center for Electron Nanoscopy

Description
Poster contribution.
Conference.

Related event
Idecat conference: Emerging challenges in catalysis
12/05/2010 → …
Porquerolles, France
Activity: Attending an event › Participating in or organising a conference

Nano Particles, Nano Structures and Near Field Computation
Period: 11 Mar 2010 → 12 Mar 2010
Mirza Karamehmedovic (Participant)
Department of Applied Mathematics and Computer Science
Scientific Computing
Department of Physics

Description
1) M. Karamehmedović, R. Schuh and V. Schmidt. Comparison of numerical methods for near-field computation
2) M. Karamehmedović. Solution of defect-detection inverse problems of Optical Diffraction Microscopy using the Method of Fundamental Solutions

Related event
Nano Particles, Nano Structures and Near Field Computation
11/03/2010 → 12/03/2010
Bremen, Germany
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Science Museum Group Journal (Journal)
Period: 1 Jan 2010 → 1 Aug 2017
Laila Zwisler (Editor)
Department of Physics

**Description**
Special Museum Theme Open Access
Degree of recognition: International
Documents:
scimusjournal201718122017_114828
Links:
http://journal.scientemuseum.org.uk/issues/autumn-2017/ (Open access journal)

**Related journal**
Science Museum Group Journal
2054-5770
Indexed in DOAJ
Local database
Activity: Research › Journal editor

**International Conference on Quantum Information Processing and Communication**
Period: 21 Sep 2009 → 25 Sep 2009
Ulrik Lund Andersen (Speaker)
Department of Physics
Quantum Physics and Information Technology

**Description**
Place: Rome, Italy

**Related external organisation**
Unknown external organisation
Activity: Talks and presentations › Conference presentations

**The eighteenth annual International Laser Physics Workshop (LPHYS'09)**
Period: 13 Jul 2009 → 17 Jul 2009
Ulrik Lund Andersen (Speaker)
Department of Physics
Quantum Physics and Information Technology

**Description**
Place: World Trade Center Barcelona
Links:
http://www.icfo.es (REL-OA)

**Related external organisation**
Unknown external organisation
Activity: Talks and presentations › Conference presentations

**Society for the History of Technology**
Period: Oct 2008
Louise Karlskov Skyggebjerg (Speaker)
Department of Physics

**Related event**
Society for the History of Technology: Annual Meeting 2008
11/10/2008 → 14/10/2008
Lisbon, Portugal
13th Nordic symposium of catalysis
Period: 5 Oct 2008
Elisabetta Maria Fiordaliso (Participant)
Department of Physics
Center for Electron Nanoscopy

Description
Oral presentation.

Conference.

Related event
13th Nordic symposium of catalysis
05/10/2008 → …
Goteborg, Sweden
Activity: Attending an event › Participating in or organising a conference

EFDA . Steering Committee (External organisation)
Period: 1 Oct 2008 → 1 Jan 2014
Jens Juul Rasmussen (Participant)
Department of Physics
Plasma Physics and Fusion Energy

Description
EFDA - European Fusion Development Association
Degree of recognition: International

Related external organisation
EFDA . Steering Committee
Activity: Membership › Membership of committees, commissions, boards, councils, associations, organisations, or similar

14th International Symposium of small particles and inorganic clusters
Period: 8 Sep 2008
Elisabetta Maria Fiordaliso (Participant)
Department of Physics
Center for Electron Nanoscopy

Description
Poster contribution.

Conference.

Related event
14th International Symposium of Small Particles and Inorganic Clusters
15/09/2008 → 19/09/2008
Valladolid, Spain
Activity: Attending an event › Participating in or organising a conference

Grand challenges of electron chemistry and catalysis at interfaces
Period: Aug 2008 → …
Elisabetta Maria Fiordaliso (Participant)
Department of Physics
We investigate the transport of non-classical light through multiple scattering random media. So far almost all experiments in the multidisciplinary field multiple light scattering have concentrated on the transport of light intensity. In recent years the quantum nature of multiple scattered light has been considered by studying the photon fluctuations of the light [1]. It was predicted that fluctuations below the classical limit can survive multiple scattering and novel spatial quantum correlations can be induced [2]. In accordance with the Heisenberg uncertainty principle, photon fluctuations smaller than the classical limit can only be generated with non-classical light sources. Using squeezed light we performed the first experimental demonstration that non-classical fluctuations survive multiple scattering of light. The experiments are in excellent agreement with theory. Moreover we demonstrate experimentally that multiple scattering induces novel spatial quantum correlations, cf. Fig. 1. Fig 1. Illustration of multiple scattering process leading to spatial quantum correlations. A non-classical light source illuminates a medium consisting of a random distribution of scatterers. The incoming light is split into a multitude of different trajectories that perform a random walk through the medium. The number of photons exiting the medium in a specific direction can be anti-correlated with the number of photons in another direction, and this correlation depends on the quantum state of light illuminating the medium.

**Related event**

**Dansk Optisk Selskabs Årsmøde 2008**
Nyborg, Denmark
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.
medium in a specific direction can be anti-correlated with the number of photons in another direction, and this correlation depends on the quantum state of light illuminating the medium.

Related event

Dansk Optisk Selskabs Årsmøde 2008
17/06/2008 → 18/06/2008
Nyborg, Denmark
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Rådgivningsgruppen for Fusionsenergi (External organisation)
Period: 1 Jun 2008 → 1 Jan 2016
Jens Juul Rasmussen (Participant)
Department of Physics
Plasma Physics and Fusion Energy

Description
Rådgivning til Forsknings og Innovationsstyrelsen vedrørende Danmarks engagement i Fusionsenergi Forskning og Udvikling

Related external organisation

Rådgivningsgruppen for Fusionsenergi

Styrelsen for Forskning og Innovation (External organisation)
Period: 15 May 2008 → …
Søren Bang Korsholm (Member)
Department of Physics
Plasma Physics and Fusion Energy

Description
Industrial Liaison Officer Network to Fusion for Energy and ITER

The F4E ILO Network is the link between the business intelligence group of F4E and European industry in preparation for tender actions with relation to ITER.

As the Danish Industrial Liaison Officer (ILO) to Fusion for Energy (F4E) the role is to be the link between the business intelligence group of F4E and Danish industry in preparation for tender actions from F4E and ITER. The ILO is part of the F4E ILO Network and participate annually in several meetings with F4E. The ILO’s are nominated by the national Governing Board members of F4E.

Body type: European
Degree of recognition: International
Links:
http://fusionforenergy.europa.eu/procurementsgrants/ilos.aspx (List of Industrial Liaison Officers to Fusion for Energy)

Related external organisation

Styrelsen for Forskning og Innovation
Denmark
Activity: Membership › Membership of committees, commissions, boards, councils, associations, organisations, or similar

Society for the History of Technology
Period: Oct 2007
Louise Karlskov Skyggebjerg (Participant)
Department of Physics
**Related event**

**Society for the History of Technology: Annual Meeting 2007**  
17/10/2007 → 21/10/2007  
Washington, United States  
Activity: Attending an event › Participating in or organising a conference

**Deutsche Physikalische Gesellschaft**  
Period: 19 Mar 2007  
Elisabetta Maria Fiordaliso (Participant)  
Department of Physics  
Center for Electron Nanoscopy  

**Description**  
Poster contribution.  
Conference.

**Related event**

**Deutsche Physikalische Gesellschaft**  
19/03/2007 → …  
Dusseldorf, Germany  
Activity: Attending an event › Participating in or organising a conference

**13th International Symposium on Small Particles and Inorganic Clusters (ISSPIC 2006)**  
Period: 2006 → …  
Elisabetta Maria Fiordaliso (Participant)  
Department of Physics  
Center for Electron Nanoscopy  

**Description**  
poster contribution  
conference

**Related event**

**13th International Symposium on Small Particles and Inorganic Clusters**  
Göteborg, Sweden  
Activity: Attending an event › Participating in or organising a conference

**EPSRC College (External organisation)**  
Period: 1 Jan 2006 → 1 Jan 2016  
Jens Juul Rasmussen (Member)  
Department of Physics  
Plasma Physics and Fusion Energy  

**Description**  
Reviewer for the UK Research Council EPSRC - Reviewing 3 applications during 2012  
Degree of recognition: International

**Related external organisation**

**EPSRC College**  
Activity: Membership › Membership of commitees, commissions, boards, councils, associations, organisations, or similar
Neutron scattering school
Period: 4 Jul 2004
Elisabetta Maria Fiordaliso (Participant)
Department of Physics
Center for Electron Nanoscopy

Description
Poster contribution.
Conference.

Related event

Neutron scattering school
04/07/2004 → …
Sirolo, Italy
Activity: Attending an event › Participating in or organising a conference

European Fusion Development Agreement (External organisation)
Period: 1 Mar 2003 → …
Søren Bang Korsholm (Participant)
Department of Physics
Plasma Physics and Fusion Energy

Description
EFDA Public Information Network
The European Fusion Development Agreement (EFDA) has a network of Public Information Officers - one from each EURATOM Fusion Association. The network assists each other and EFDA in the dissemination of information about fusion energy research to the public.

Body type: European network
Degree of recognition: International
Links:
http://www.efda.org (EFDA website)

Related external organisation

European Fusion Development Agreement
Activity: Membership › Membership of committees, commissions, boards, councils, associations, organisations, or similar

Physica Scripta (Journal)
Period: 1 Jan 1998 → 1 Jan 2020
Jens Juul Rasmussen (Editor)
Department of Physics
Plasma Physics and Fusion Energy

Description
International journal for Physics
Topical editor : Plasma Physics, Nonlinear Dynamics; General Physics

Related journal

Physica Scripta
0031-8949
Central database
Activity: Research › Journal editor
Topical Editor Physica Scripta (External organisation)
Period: 1 Jan 1998 → 1 Jan 2020
Jens Juul Rasmussen (Participant)
Department of Physics
Plasma Physics and Fusion Energy

Description
Topical Editor at the Journal Physica Scripta
Degree of recognition: International

Related external organisation

Prizes:

Best talk at DFS 2016
Jesper Rasmussen (Recipient)
Department of Physics, Plasma Physics and Fusion Energy

Description
Award for "Best talk" (DKK 2500) at the Annual Meeting of the Danish Physical Society 2016

Details
Awarded date: 7 Jun 2016
Degree of recognition: National
Granting Organisations: Danish Physical Society
Prize: Prizes, scholarships, distinctions

First Prize Reach.Out! 2015
Anne Hansen (Recipient)
Department of Physics

Description

Details
Awarded date: 13 May 2015
Granting Organisations: European Materials Research Society (E-MRS)
Prize: Prizes, scholarships, distinctions

Press clippings:

Deltagelse i radioprogrammet Dommedag aflyst 3:4 - Teknologiens potentiale
Louise Karlskov Skyggebjerg
07/04/2018
Department of Physics

Media contribution (1)

Dommedag aflyst 3:4 - Teknologiens potentiale
07/04/2018
P1 (National), Denmark, Radio
Liv Thomsen
Artikel på DR.dk om fusionsenergi
Søren Bang Korsholm
30/01/2018
Department of Physics, Plasma Physics and Fusion Energy

Media contribution (1)

En kunstig sol og helium fra Månen: Sådan vil forskerne revolutionere energiproduktion
30/01/2018
Danmarks Radio (National), Denmark, Web
JEPPE KYHNE KNUDSEN, JONAS PETRI OG LASSE FROM, DR Viden
Webartikel (~2-3 A4 sider) samt video
Søren Bang Korsholm
Press / Media

"Finn Foton og kvantefysikken" i nyhederne på TV2 Østjylland
Ulrich Busk Hoff
09/01/2018
Quantum Physics and Information Technology, Department of Physics

Media coverage (1)

Nyhederne, TV2 Østjylland
09/01/2018
TV2 Østjylland (National), Denmark, Television
https://www.tv2ostjylland.dk/artikel/boern-i-3-klasse-laerer-om-kvantefysik-det-er-ret-sejt
Ulrich Busk Hoff
Press / Media

Interview til Ren og evig energi: Kunstig intelligens skal hjælpe med at lave en sol på Jorden
Søren Bang Korsholm
30/12/2017
Department of Physics, Plasma Physics and Fusion Energy

Media contribution (1)

Ren og evig energi: Kunstig intelligens skal hjælpe med at lave en sol på Jorden
30/12/2017
Politiken (National), Denmark, Print
Mathias Glistrup, Politiken
1 full page in print and online
https://politiken.dk/viden/art6271411/Kunstig-intelligens-skal-hj%C3%A6lpe-med-at-lave-en-sol-p%C3%A5-Jorden
Søren Bang Korsholm
Press / Media

Deltagelse i podcast Industri på udstilling
Louise Karlskov Skyggebjerg
07/12/2017
Department of Physics

Media contribution (1)

Industri på udstilling - podcast
07/12/2017
Denmark, Other
Christoffer Heide Høyer
https://unipress.dk/bogserier/100-danmarkshistorier/
Louise Karlskov Skyggebjerg
Press / Media

"Finn Foton og kvantefysikken" i 22 Nyhederne på TV2
Ulrich Busk Hoff
27/11/2017
Quantum Physics and Information Technology, Department of Physics

Media coverage (1)

22 Nyhederne
27/11/2017
TV2 (National), Denmark, Television
Ulrich Busk Hoff
Press / Media

Kvantemekanik skal være allemandseje
Ulrich Busk Hoff
29/04/2017
Quantum Physics and Information Technology, Department of Physics

Media coverage (1)

Kvantemekanik skal være allemandseje
29/04/2017
Ingeniøren (National), Denmark, Web
Kristian Balle Ravn
https://ing.dk/artikel/kvantemekanik-skal-vaere-allemandseje-197695
Ulrich Busk Hoff
Press / Media

Ugens Podcast: Kan du forstå kvantefysik?
Ulrich Busk Hoff
12/04/2017
Quantum Physics and Information Technology, Department of Physics

Media contribution (1)

Ugens Podcast: Kan du forstå kvantefysik?
12/04/2017
ForskerZonen/Videnskab.dk (National), Denmark, Web
Camilla Segaard Kristensen
19:54
http://videnskab.dk/naturvidenskab/ugens-podcast-kan-du-forstaa-kvantefysik
Ulrich Busk Hoff
Press / Media

Hvordan formidler vi kvantefysik, vi ikke kan se?
Ulrich Busk Hoff
12/04/2017
Quantum Physics and Information Technology, Department of Physics

Media contribution (1)

Hvordan formidler vi kvantefysik, vi ikke kan se?
12/04/2017
ForskerZonen/Videnskab.dk (National), Denmark, Web
Ulrich Busk Hoff
http://videnskab.dk/naturvidenskab/hvordon-formidler-vi-kvantefysik-vi-ikke-kan-se
Ulrich Busk Hoff
Press / Media
Interview i DR2 Dagen om fusionsenergi, CPH|DOX og Let there be light
Søren Bang Korsholm
27/03/2017
Department of Physics, Plasma Physics and Fusion Energy

Media contribution (1)

Interview i DR2 Dagen om fusionsenergi, CPH|DOX og Let there be light
27/03/2017
Danmarks Radio DR2 (National), Denmark, Television
15 minutter
http://www.dr.dk/tv/se/dr2-dagen-tv/dr2-dagen-2017-03-27#!/
Søren Bang Korsholm
Press / Media

Fysiker vil hverve unge til kvanteforskningen
Ulrich Busk Hoff
06/03/2017
Quantum Physics and Information Technology, Department of Physics

Media contribution (1)

Fysiker vil hverve unge til kvanteforskningen
06/03/2017
Videnskab.dk (National), Denmark, Web
Johanne Uhrenholt Kusnitzoff
http://videnskab.dk/naturvidenskab/fysiker-vil-hverve-unge-til-kvanteforskningen
Ulrich Busk Hoff
Press / Media

Kom med kvantemekanikkens skyggejægere i laboratoriet
Ulrich Busk Hoff & Christian Scheffmann Jacobsen
07/01/2017
Quantum Physics and Information Technology, Department of Physics

Media contribution (1)

Kom med kvantemekanikkens skyggejægere i laboratoriet
07/01/2017
Videnskab.dk (National), Denmark, Web
Johanne Uhrenholt Kusnitzoff
http://videnskab.dk/naturvidenskab/kom-med-kvantemekanikkens-skyggejaegere-i-laboratoriet
Ulrich Busk Hoff & Christian Scheffmann Jacobsen
Department of Physics, Quantum Physics and Information Technology
Press / Media

Her jagter forskerne nøglen til kvantecomputeren
Ulrich Busk Hoff
12/11/2016
Quantum Physics and Information Technology, Department of Physics

Media contribution (1)

Her jagter forskerne nøglen til kvantecomputeren
12/11/2016
Ingeniøren (National), Denmark, Web
Jens Ramskov
https://ing.dk/artikel/her-jagter-forskerne-noglen-kvantecomputeren-188154
Ulrich Busk Hoff
Press / Media

DTU inviterer gymnasieelever og andet godtfolk til at lave kvanteeeksperimenter
Ulrich Busk Hoff
DTU inviterer gymnasieelever og andet godtfolk til at lave kvanteeksperimenter
09/11/2016
Ingeniøren (National), Denmark, Web
Jens Ramskov
https://ing.dk/artikel/dtu-inviterer-gymnasieelever-andet-godtfolk-at-lave-kvanteeksperimenter-187928
Ulrich Busk Hoff
Press / Media

Dansk professor får prestigefuld toppost i Hamborg
Martin Meedom Nielsen
17/10/2016
Department of Physics, Neutrons and X-rays for Materials Physics

Der beste Laser der Welt
Martin Meedom Nielsen
06/10/2016
Department of Physics, Neutrons and X-rays for Materials Physics

Sommertema i DR P1 Orientering
Søren Bang Korsholm
18/07/2016
Description
http://www.dr.dk/radio/ondemand/p1/orientering-2016-07-18/#!01:00:11
Søren Bang Korsholm was one of three scientists being interviewed about current and status of science. Department of Physics, Plasma Physics and Fusion Energy

Sommertema i DR P1 Orientering
18/07/2016
DR, Radio
Chris Lehmann
53 minutes
http://www.dr.dk/radio/ondemand/p1/orientering-2016-07-18/#!01:00:11
Direct link to 53 minutes interview at DR P1
Søren Bang Korsholm
Department of Physics, Plasma Physics and Fusion Energy
Press / Media
Interview i TV2 News - New Science - om Viborg Mercantec fusoren: Indslag i forbindelse med Viborg Tekniske Gymnasiums åbningsceremoni for deres fusor
Søren Bang Korsholm
28/04/2016

Subject
I forbindelse med Viborg Tekniske Gymnasiums åbningsceremoni for deres fusor
Department of Physics, Plasma Physics and Fusion Energy

Media contribution (1)

Interview i TV2 News - New Science - om Viborg Mercantec fusoren: Indslag i forbindelse med Viborg Tekniske Gymnasiums åbningsceremoni for deres fusor
28/04/2016
TV2 News, Television
5 minutter
Søren Bang Korsholm
Department of Physics, Plasma Physics and Fusion Energy
Press / Media

Interview i TV2 Nyhederne med Skammelsen: TV2s 22-Nyhederne med Poul Erik Skammelsen
Søren Bang Korsholm
28/04/2016

Subject
Indslaget var indledt med en rapport fra dagens åbning af fusoren i Viborg Tekniske Gymnasium og afsluttedes med et interview i Skammelsens studie af Søren Bang Korsholm.
Emnet var uddannelse og behov for teknisk- og naturvidenskabeligt interesserede unge med udgangspunkt i dagens åbningsceremoni for Viborg Tekniske Gymnasiums fusor.
Department of Physics, Plasma Physics and Fusion Energy

Media contribution (1)

Interview i TV2 Nyhederne med Skammelsen: TV2s 22-Nyhederne med Poul Erik Skammelsen
28/04/2016
TV2, Television
Michael Malling Loehr
5 minutter
Søren Bang Korsholm
Department of Physics, Plasma Physics and Fusion Energy
Press / Media

Fuld fart på forskningen i fusionskraft: Interview på videnskab.dk
Søren Bang Korsholm
09/12/2015

Subject
Statusartikel om fusionsforskningen.
Department of Physics, Plasma Physics and Fusion Energy

Media contribution (1)

Fuld fart på forskningen i fusionskraft: Interview på videnskab.dk
09/12/2015
videnskab.dk, Web
Henrik Bendix
http://videnskab.dk/teknologi/fuld-fart-pa-forskningen-i-fusionskraft
Søren Bang Korsholm
Department of Physics, Plasma Physics and Fusion Energy
Press / Media
Kvantemekanik bruges til super sikker kommunikation: Kvantemekanikken fører til nye kommunikationsmetoder, der forhindre hacking. Forskere fra York og DTU har introduceret en ny teknik der tåler infiltration af måleudstyret.
Christian Scheffmann Jacobsen
11/06/2015

Hjemmekraftværk rammer tidens ånd
Tejs Vegge
04/05/2015

Nyt batteri kan forsyne dit hus med strøm
Tejs Vegge
01/05/2015

Nyt batteri kan forsyne dit hus med strøm
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

Besøg på DTU's historiske samling
Laila Zwisler
13/03/2015

Subject
Opfindelsernes historie
Department of Physics

Media contribution (1)

Besøg på DTU's historiske samling
13/03/2015
P1, Radio
5 minutter
http://www.dr.dk/p1/p1-ettermiddag/p1-ettermiddag-2015-03-13
Link to interview
Laila Zwisler
Department of Physics

DTU får kæmpeordre på avanceret måleudstyr til fusionsreaktor
Søren Bang Korsholm
20/02/2014

Subject
Artikl om den nyvundne F4E kontrakt på design af CTS systemet til ITER
Department of Physics, Plasma Physics and Fusion Energy

Media contribution (1)

DTU får kæmpeordre på avanceret måleudstyr til fusionsreaktor
20/02/2014
Ingeniøren, Print
Jens Ramskov
https://ing.dk/artikel/dtu-faar-kaempeordre-paa-avanceret-maaleudstyr-til-fusionsreaktor-166454
Søren Bang Korsholm
Department of Physics, Plasma Physics and Fusion Energy
Press / Media
Danske fysikere åbner vindue til processerne i Solens kerne
Søren Bang Korsholm
19/02/2014

Subject
Artikel både i Berlingske Tidende (trykt udgave) og på b.dk
Department of Physics, Plasma Physics and Fusion Energy

Media contribution (1)

Danske fysikere åbner vindue til processerne i Solens kerne
19/02/2014
Berlingske Tidende, Print
http://www.b.dk/nationalt/danske-fysikere-aabner-vindue-til-processerne-i-solens-kerne
Søren Bang Korsholm
Department of Physics, Plasma Physics and Fusion Energy

Forskere vil revolutionere informationssamfundet
Ulrich Busk Hoff
07/01/2013
Quantum Physics and Information Technology, Department of Physics

Media contribution (1)

Forskere vil revolutionere informationssamfundet
07/01/2013
www.videnskab.dk, Web
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Derfor liv på jorden og ikke på Venus
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