Decomposition of formic acid over silica encapsulated and amine functionalised gold nanoparticles

Formic acid has recently attracted considerable attention as a safe and convenient source of hydrogen for sustainable chemical synthesis and renewable energy storage. Here, we show that silica encapsulated and amine functionalised gold nanoparticles are highly active catalysts for the production of hydrogen by vapour phase decomposition of formic acid. The core-shell catalysts are prepared in a reverse micelle system that makes it possible to control the size of the Au nanoparticles and the thickness of the SiO2 shells, which has a large impact on the catalytic activity. The smallest gold nanoparticles are 2.2 ± 0.3 nm in diameter and have a turnover frequency (TOF) of up to 958 h⁻¹ at a temperature of 130 °C. Based on detailed in situ ATR-FTIR studies and results from kinetic isotope labelling experiments we propose that the active site is a low-coordinated and amine functionalised Au atom, while H-assisted formate decomposition into CO₂ and H₂ is the rate limiting step.
Nitrogen-Doped Carbon Encapsulated Nickel/Cobalt Nanoparticle Catalysts for Olefin Migration of Allylarenes

Olefin migration of allylarenes is typically performed with precious metal-based homogeneous catalysts. In contrast, very limited progress has been made using cheap, earth-abundant base metals as heterogeneous catalysts for these transformations - in spite of the obvious economic and environmental advantages. Herein, we report on the use of an easily prepared heterogeneous catalyst material for the migration of olefins, in particular allylarenes. The catalyst material consists of nickel/cobalt alloy nanoparticles encapsulated in nitrogen-doped carbon shells. The encapsulated nanoparticles are stable in air and easily collected by centrifugation, filtration, or magnetic separation. Furthermore, we demonstrate that the catalysts can be reused several times providing continuously high yields of the olefin migration product.

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry, Center for Electron Nanoscopy
Efficient Production of Hydrogen from Decomposition of Formic Acid over Zeolite Incorporated Gold Nanoparticles

Formic acid has a great potential as a safe and convenient source of hydrogen for sustainable chemical synthesis and renewable energy storage. Here, we report a heterogeneous gold nanoparticles catalyst for efficient production of hydrogen from vapor phase decomposition of formic acid using zeolite incorporated gold nanoparticles. The catalyst is prepared by pressure assisted impregnation and reduction (PAIR), which results in a uniform distribution of small gold nanoparticles that are incorporated into zeolite silicalite-1 crystals. Consequently, the incorporated nanoparticles exhibit increased sintering stability. Based on these results, we believe that incorporation of metal nanoparticles in zeolites may find use as highly active and selective heterogeneous catalysts for the production of hydrogen in future renewable energy applications.

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry
Authors: Gallas-Hulin, A. (Intern), Mielby, J. J. (Intern), Kegnæs, S. (Intern)
Number of pages: 4
Pages: 3942-3945
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: ChemistrySelect
Volume: 1
Lignin biomass conversion into chemicals and fuels

Second-generation biomass or lignocellulosic biomass, which is mainly composed of cellulose, hemicellulose and lignin, is a very important and promising feedstock for the renewable production of fuels and chemicals of the future. Lignin is the second most abundant natural polymer, representing 30% of the weight and 40% of the energy content of lignocellulosic biomass. While designated applications for cellulose already exist in form of the current pulp and paper production as well as its prospective hydrolysis and fermentation into biofuels (mainly bioethanol), sustainable ways to valorize the lignin fraction of wood are yet to be established, due to its poor solubility and complex heterogeneous structure. This constitutes a major drawback in the economic viability of a biorefinery, where complete valorization of lignocellulosic biomass is necessary. For this reason, and due to its potential as a valuable feedstock for the production of organic chemicals, lignin valorization has become an important issue to solve.

For a better understanding and analysis of the catalytic performance of lignin, it is common to use lignin model compounds, which contain the most significant linkages present in lignin and show similar, although simplified, characteristics to the natural biopolymer. Among them, the most abundant structural unit is the β-O-4, representing approximately 60% of the bonds in hardwood and 45-50% of those in softwood.

Oxidative depolymerization is one of the most viable methods for lignin valorization. It involves the cleavage of ether bonds, such as β-O-4 and other linkages present in lignin and its model compounds, giving aldehydes or carboxylic acids as products, depending on the reaction conditions used. In Chapter 2 of this thesis, the preparation, characterization and catalytic performance of heterogeneous catalysts for the aerobic oxidation of β-O-4 lignin model compounds (veratryl alcohol and guaiacyl glycerol-β-guaiacyl ether) is discussed. The use of an environmentally friendly process, the organosolv process, for treating lignocellulosic biomass in the presence of a solvent and using reaction conditions under which at least part of the lignin is separated from the biomass, is described in Chapter 3. Different catalysts and reaction conditions have been studied in order to optimize the organosolv process for the production of high-quality lignin for further upgrading.

At the end of this thesis, Chapter 4, a catalytic process is described for the valorization of lignin, consisting of a two-step catalytic system. The two-step catalytic system involved catalytic oxidation, followed by hydrogenolysis. A catalytic system was developed for lignin hydrogenolysis and the influence of the temperature and reaction time was studied for the catalytic oxidation of lignin.

The results presented in this thesis contribute to a better understanding of the various factors influencing the production of bulk aromatic chemicals from lignin, including valuable knowledge regarding catalyst activity and stability, optimal conditions for the valorization of lignin and lignin model compounds, and a process for the extraction of lignin from wood. Hence, it is necessary to further develop catalytic processes to enable the transformation of lignin from a low quality, low-price waste product into a high-quality, high-value feedstock for bulk and specialty chemicals by the development of the appropriate catalytic technology. This transformation is critical because lignin represents the only viable renewable source to produce the aromatic compounds on which society currently depends.

General information
State: Published
Organisations: Organic Chemistry, Department of Chemistry; Centre for Catalysis and Sustainable Chemistry
Authors: Mélia Rodríguez, M. (Intern), Riisager, A. (Intern), Kegnæs, S. (Intern), Shunmugavel, S. (Intern)
Number of pages: 158
Publication date: 2016

Publication information
Publisher: DTU Chemistry
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
Lignin biomass conversion

Relations
Projects:
Lignin biomass conversion into chemicals and fuels
Mesoporous MEL, BEA, and FAU zeolite crystals obtained by in situ formation of carbon template over metal nanoparticles

Here, we report the synthesis and characterization of hierarchical zeolite materials with MEL, BEA and FAU structures. The synthesis is based on the carbon templating method with an in situ-generated carbon template. Through the decomposition of methane and deposition of coke over nickel nanoparticles supported on silica, a carbon–silica composite is obtained and exploited as a combined carbon template/silica source for the zeolite synthesis. The mesoporous zeolite materials were all prepared by hydrothermal crystallization in alkaline media followed by removal of the carbon template by combustion, which results in zeolite single crystals with intracrystalline pore volumes of up to 0.44 cm$^3$ g$^{-1}$. The prepared zeolite structures are characterized by XRD, SEM, TEM and N$_2$ physisorption measurements.

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry, Technical University of Denmark, Haldor Topsoe AS
Authors: Abildstrøm, J. O. (Intern), Ali, Z. N. (Ekstern), Mentzel, U. V. (Ekstern), Mielby, J. J. (Intern), Kegnæs, S. (Intern), Kegnæs, M. (Ekstern)
Number of pages: 5
Pages: 4223-4227
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: New Journal of Chemistry
Volume: 40
Issue number: 5
ISSN (Print): 1144-0546
Ratings:
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.08 SJR 0.869 SNIP 0.766
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.954 SNIP 0.836 CiteScore 3.27
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.01 SNIP 0.872 CiteScore 3.14
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.047 SNIP 0.838 CiteScore 3.03
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.209 SNIP 0.825 CiteScore 2.8
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.148 SNIP 0.81 CiteScore 2.66
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.282 SNIP 0.852
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.366 SNIP 0.899
Synthesis of mesoporous zeolite catalysts by in situ formation of carbon template over nickel nanoparticles

A novel synthesis procedure for the preparation of the hierarchical zeolite materials with MFI structure based on the carbon templating method with in situ generated carbon template is presented in this study. Through chemical vapour deposition of coke on nickel nanoparticles supported on silica oxide, a carbon-silica composite is obtained and exploited as a combined carbon template/silica source for zeolite synthesis. This approach has several advantages in comparison with conventional carbon templating methods, where relatively complicated preparative strategies involving multistep impregnation procedures and rather expensive chemicals are used. Removal of the carbon template by combustion results in zeolite single crystals with intracrystalline pore volumes between 0.28 and 0.48 cm$^3$/g. The prepared zeolites are characterized by XRD, SEM, TEM and physisorption analysis. The isomerization and cracking of n-octane is chosen as a model test reaction and the mesoporous zeolite catalyst is found to exhibit higher activity than the conventional catalyst.
A general method to incorporate metal nanoparticles in zeolites and zeotypes

Disclosed herein is a method for producing a zeolite, zeolite-like or zeotype structure with selective formation of metal, metal oxide or metal sulphide nanoparticles and/or clusters inside the zeolite, zeolite-like or zeotype structure.

General information
State: Published
Organisations: Technical University of Denmark, Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry
Authors: Kegnæs, S. (Intern), Mielby, J. J. (Intern), Abildstrøm, J. O. (Intern)
Publication date: 15 Oct 2015

Publication information
IPC: B01J 29/ 035 A I
Patent number: WO2015155216
Date: 15/10/2015
Priority date: 10/04/2014
Priority number: EP20140164188
Original language: English
Electronic versions:
WO2015155216A1.pdf
Main Research Area: Technical/natural sciences
Source: espacenet
Aerobic Oxidation of Veratryl Alcohol to Veratraldehyde with Heterogeneous Ruthenium Catalysts

Lignin is a complex polymeric molecule constituting various linkages between aromatic moieties. Typically, the β-O-4 linkage accounts for more than half of the linkage structures present in lignin. The current study focuses on the oxidative transformation of veratryl alcohol (VA)—a compound that can be formed by cleavage of β-O-4 linkages in lignin—to veratraldehyde (VAld) with air using ruthenium supported on γ-alumina or silica as catalyst with water or methanol as solvent in a batch reactor. Ru/Al₂O₃, prepared with ruthenium(IV)oxide hydrate showed superior catalytic activity, yielding 89 % VAld in water at 160 °C with 5 bar air pressure after 8 h of reaction. Prolonged reaction time led to significant formation of the decarbonylated product veratrol from VAld. When the reaction was completed under 20 bars of argon in methanol instead of water, the methyl ether of VA (i.e. 1,2-dimethoxy-4-(methoxymethyl)benzene) prevailed, indicating that methanol protected the hydroxyl group in VA from being oxidized to VAld. Catalysts containing alternative transition metals (Mn, Co, Cu and Ag) supported on Al₂O₃ gave significantly lower activities compared to Ru/Al₂O₃ under identical reaction conditions. The Ru/Al₂O₃ catalyst was reused in three consecutive reaction runs in water, but a decrease in VAld yield was obtained after the third cycle possibly due to leaching of Ru from the support.

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry
Authors: Melián Rodriguez, M. (Intern), Shunmugavel, S. (Intern), Kegnæs, S. (Intern), Riisager, A. (Intern)
Number of pages: 7
Pages: 1036-1042
Publication date: Oct 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Topics in Catalysis
Volume: 58
Issue number: 14
ISSN (Print): 1022-5528
Ratings:
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.974 SNIP 0.878 CiteScore 2.55
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.945 SNIP 0.789 CiteScore 2.41
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.989 SNIP 0.862 CiteScore 2.29
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.125 SNIP 0.837 CiteScore 2.67
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.196 SNIP 0.851 CiteScore 2.49
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.346 SNIP 0.977 CiteScore 2.89
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.492 SNIP 0.91
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Aerobic oxidation of β-O-4 lignin model compounds with solid catalysts

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry
Authors: Melián Rodríguez, M. (Intern), Shunmugavel, S. (Intern), Kegnæs, S. (Intern), Riisager, A. (Intern)
Publication date: 2015
Event: Abstract from COST Action Meeting, Belgrade, Serbia.
Main Research Area: Technical/natural sciences
Electronic versions:
COST_Abstract_MAYRA_MELIAN.pdf

Relations
Activities:
COST Action Lignoval
Publication: Research - peer-review » Conference abstract for conference – Annual report year: 2015

Catalytic oxidation of lignin and lignin model compounds

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry
Authors: Melián Rodríguez, M. (Intern), Shunmugavel, S. (Intern), Kegnæs, S. (Intern), Riisager, A. (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
Catalytic oxidation of veratryl alcohol – a β-O-4 lignin model compound - to veratraldehyde

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry
Authors: Melián Rodríguez, M. (Intern), Shunmugavel, S. (Intern), Kegnæs, S. (Intern), Riisager, A. (Intern)
Number of pages: 2
Publication date: 2015
Main Research Area: Technical/natural sciences
Electronic versions:
MAYRA_ABSTRACT_EuropaCat_Final.pdf

Relations
Activities:
12th European Congress on Catalysis
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2015

Catalytic oxidation of veratryl alcohol – a β-O-4 lignin model compound – to veratraldehyde

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry
Authors: Melián Rodríguez, M. (Intern), Shunmugavel, S. (Intern), Kegnæs, S. (Intern), Riisager, A. (Intern)
Publication date: 2015
Main Research Area: Technical/natural sciences
Electronic versions:
Europacat_poster_FINAL.pdf

Relations
Activities:
12th European Congress on Catalysis
Publication: Research - peer-review › Poster – Annual report year: 2015

Conversion of lignin into chemicals with heterogeneous catalysis: Current and future technologies

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry
Authors: Melián Rodríguez, M. (Intern), Shunmugavel, S. (Intern), Kegnæs, S. (Intern), Riisager, A. (Intern)
Publication date: 2015
Event: Poster session presented at 2nd International Congress on Catalysis for Biorefineries, Dalian, China.
Main Research Area: Technical/natural sciences
Electronic versions:
Lignin_poster.pdf

Relations
Activities:
2nd International Congress on Catalysis for Biorefineries
Publication: Research - peer-review › Poster – Annual report year: 2013
Conversion of lignin into chemicals with heterogeneous catalysis: Current and future technologies

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry
Authors: Melián Rodríguez, M. (Intern), Shunmugavel, S. (Intern), Kegnæs, S. (Intern), Riisager, A. (Intern)
Number of pages: 2
Publication date: 2015
Event: Abstract from 2nd International Congress on Catalysis for Biorefineries, Dalian, China.
Main Research Area: Technical/natural sciences
Electronic versions:
Catalytic_conversion_lignin_Abstract.pdf

Relations
Activities:
2nd International Congress on Catalysis for Biorefineries
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2013

Heterogeneous catalysis in oxidation of lignin model compounds

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry
Authors: Melián Rodríguez, M. (Intern), Shunmugavel, S. (Intern), Kegnæs, S. (Intern), Riisager, A. (Intern)
Publication date: 2015
Main Research Area: Technical/natural sciences
Electronic versions:
nordicabstract_MAYRA.pdf

Relations
Activities:
16th Nordic Symposium on Catalysis
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2014

Heterogeneous catalysis in oxidation of lignin model compounds

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry
Authors: Melián Rodríguez, M. (Intern), Shunmugavel, S. (Intern), Kegnæs, S. (Intern), Riisager, A. (Intern)
Publication date: 2015
Main Research Area: Technical/natural sciences
Electronic versions:
nordic.pdf

Relations
Activities:
16th Nordic Symposium on Catalysis
Publication: Research › Poster – Annual report year: 2014

Lignin Valorization by Heterogeneous Catalytic Oxidation

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry
Authors: Melián Rodríguez, M. (Intern), Shunmugavel, S. (Intern), Kegnæs, S. (Intern), Riisager, A. (Intern)
Publication date: 2015
Main Research Area: Technical/natural sciences
Lignin Valorization using Heterogeneous Catalytic Oxidation

The research interests in biomass conversion to fuels and chemicals has increased significantly in the last decade in view of current problems such as global warming, high oil prices, food crisis and other geopolitical scenarios. Many different reactions and processes to convert biomass into high-value products and fuels have been proposed in the literature, giving special attention to the conversion of lignocellulosic biomass, which does not compete with food resources and is widely available as a low cost feedstock. Lignocellulose biomass is a complex material composed of three main fractions: cellulose (40-50%), hemicellulose (25-35%) and lignin (20-30%). Lignin is mainly composed of three different monolignol monomers: p-coumaryl, coniferyl and sinapyl alcohol. These monomers are connected with various linkages with the most common one being the ß-O-4 linkage. The lignin structure is complex so different model compounds are often used to study lignin valorization. These model compounds contain the linkages present in lignin, simplifying catalytic analysis and present analytical challenges related to the study of the complicated lignin polymer and the plethora of products that could be obtained. Heiko Lange et al., has reported that the catalytic oxidation products of lignin and lignin model compounds range from aromatic aldehyde and carboxylic acid and they must be originate from oxidation of side chain. The products we obtained in these reactions are based on the severity of the reaction conditions. Here, we therefore present an overview of the recent research about conversion of some lignin model compounds using heterogeneous catalysis in oxidation reactions.

Method for producing zeolites and zeotypes

The invention relates to a method for producing zeolite, zeolite-like or zeotype particles comprising the steps of: 1) Adding one or more metal precursors to a silica or alumina source; 2) Reducing the one or more metal precursors to form metal nanoparticles on the surface of the silica or alumina source; 3) Passing a gaseous hydrocarbon, alkyl alcohol or alkyl ether over the silica or alumina supported metal nanoparticle to form a carbon template coated zeolite, zeolite-like or zeotype precursor composition; 4a) Adding a structure directing agent to the carbon template coated zeolite, zeolite-like or zeotype precursor composition thereby creating a zeolite, zeolite-like or zeotype gel composition; 4b) Crystallising the zeolite, zeolite-like or zeotype gel composition by subjecting said composition to a hydrothermal treatment; 5) Removing the carbon template and structure directing agent and isolating the resulting zeolite, zeolite-like or zeotype particles.
Method of producing zeolite encapsulated nanoparticles.

The invention therefore relates to a method for producing zeolite, zeolite-like or zeotype encapsulated metal nanoparticles, the method comprises the steps of: 1) Adding one or more metal precursors to a silica or alumina source; 2) Reducing the one or more metal precursors to form metal nanoparticles on the surface of the silica or alumina source; 3) Passing a gaseous hydrocarbon, alkyl alcohol or alkyl ether over the silica or alumina supported metal nanoparticles to form a carbon template coated zeolite, zeolite-like or zeotype precursor composition; 4a) Adding a structure directing agent to the carbon template coated zeolite, zeolite-like or zeotype precursor composition thereby creating a zeolite, zeolite-like or zeotype gel composition; 4b) Crystallising the zeolite, zeolite-like or zeotype gel composition by subjecting said composition to a hydrothermal treatment; 5) Removing the carbon template and structure directing agent and isolating the resulting zeolite, zeolite-like or zeotype encapsulated metal nanoparticles.
A Polyphenylene Support for Pd Catalysts with Exceptional Catalytic Activity

We describe a solid polyphenylene support that serves as an excellent platform for metal-catalyzed reactions that are normally carried out under homogeneous conditions. The catalyst is synthesized by palladium-catalyzed Suzuki coupling which directly results in formation of palladium nanoparticles confined to a porous polyphenylene network. The composite solid is in turn highly active for further Suzuki coupling reactions, including non-activated substrates that are challenging even for molecular catalysts.
Formation of pyridine N-oxides using mesoporous titanium silicalite-1

Mesoporous titanium silicalite-1 (TS-1) prepared by carbon-templating is significantly more active than conventional TS-1 for the oxidation of pyridine derivatives using aqueous hydrogen peroxide as oxidant. The catalytic activity is increased by the system of meso pores that helps to overcome the configurational diffusion limitations within the microporous catalyst.
The use of a carbon-template for generation of secondary porosity is more effective than desilication. The desilicated catalyst is slightly more active than conventional TS-1, probably due to a decrease of the mean diffusion path length. In contrast, carbon-templated mesopores provides an efficient transport throughout the zeolite, thus preventing deactivation due to product confinement. All catalysts were characterised by X-ray powder diffraction, scanning electron microscopy, UV-Vis spectroscopy and nitrogen physisorption. The results indicate that desilication may cause a surface densification of less catalytically active extra-framework Ti species. Carbon-templating is thus a more gentle and effective method for generating secondary porosity. Utilization of carbon-templated mesoporous TS-1 for oxidation of pyridine derivatives represents a new and environmentally friendly method to synthesise N-oxides.

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Department of Chemistry, Centro de Investigaciones Biologicas
Authors: Mielby, J. J. (Intern), Abildstrøm, J. O. (Intern), Perez-Ferreras, S. (Ekstern), Rasmussen, S. B. (Intern), Kegnæs, S. (Intern)
Pages: 531-537
Publication date: 2014
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Porous Materials
Volume: 21
Issue number: 5
ISSN (Print): 1380-2224
Ratings:
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.483 SNIP 0.679 CiteScore 1.59
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.404 SNIP 0.615 CiteScore 1.32
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.462 SNIP 0.735 CiteScore 1.44
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.497 SNIP 0.884 CiteScore 1.5
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.522 SNIP 0.977 CiteScore 1.35
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.538 SNIP 0.85 CiteScore 1.33
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.418 SNIP 0.465
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.455 SNIP 0.527
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.448 SNIP 0.496
Scopus rating (2007): SJR 0.481 SNIP 0.634
Scopus rating (2006): SJR 0.435 SNIP 0.59
Scopus rating (2005): SJR 0.383 SNIP 0.621
Scopus rating (2004): SJR 0.441 SNIP 0.764
Scopus rating (2003): SJR 0.428 SNIP 0.673
Scopus rating (2002): SJR 0.489 SNIP 0.552
Scopus rating (2001): SJR 0.582 SNIP 0.762
Scopus rating (2000): SJR 0.547 SNIP 0.963
Scopus rating (1999): SJR 0.573 SNIP 1.008
Highly selective formation of imines catalyzed by silver nanoparticles supported on alumina

The oxidative dehydrogenation of alcohols to aldehydes catalyzed by Ag nanoparticles supported on Al2O3 was studied. The catalyst promoted the direct formation of imines by tandem oxidative dehydrogenation and condensation of alcohols and amines. The reactions were performed under mild conditions and afforded the imines in high yield (up to 99%) without any byproducts other than H2O. The highest activity was obtained over 5 wt% Ag/Al2O3 in toluene with air as oxidant. The reactions were also performed under oxidant-free conditions where the reaction was driven to the product side by the production of H-2 in the gas phase. The use of an efficient and selective Ag catalyst for the oxidative dehydrogenation of alcohol in the presence of amines gives a new green reaction protocol for imine synthesis. (C) 2014, Dalian Institute of Chemical Physics, Chinese Academy of Sciences. Published by Elsevier B.V. All rights reserved.
Lignin valorization using heterogeneous catalytic oxidation

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry
Authors: Melián Rodríguez, M. (Intern), Shunmugavel, S. (Intern), Kegnæs, S. (Intern), Riisager, A. (Intern)
Number of pages: 1
Publication date: 2014
Event: Poster session presented at Summer School on Catalysis of Biomass, Liblice, Czech Republic.
Main Research Area: Technical/natural sciences
Electronic versions:
Mayra_Biomass_SummerSchool_Poster.pdf

Oxidation of Bioethanol using Zeolite-Encapsulated Gold Nanoparticles

With the ongoing developments in biomass conversion, the oxidation of bioethanol to acetaldehyde may become a favorable and green alternative to the preparation from ethylene. Here, a simple and effective method to encapsulate gold nanoparticles in zeolite silicalite-1 is reported and their high activity and selectivity for the catalytic gas-phase oxidation of ethanol are demonstrated. The zeolites are modified by a recrystallization process, which creates intraparticle voids and mesopores that facilitate the formation of small and disperse nanoparticles upon simple impregnation. The individual zeolite crystals comprise a broad range of mesopores and contain up to several hundred gold nanoparticles with a diameter of 2–3 nm that are distributed inside the zeolites rather than on the outer surface. The encapsulated nanoparticles have good stability and result in 50 % conversion of ethanol with 98 % selectivity toward acetaldehyde at 200 °C, which (under the given reaction conditions) corresponds to 606 mol acetaldehyde/mol Au hour−1.

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Center for Electron Nanoscopy, Max-Planck-Institut für Kohlenforschung
Authors: Mielby, J. J. (Intern), Abildstrøm, J. O. (Intern), Wang, F. (Ekstern), Kasama, T. (Intern), Weidenthaler, C. (Ekstern), Kegnæs, S. (Intern)
Pages: 12721 –12724
Publication date: 2014
Main Research Area: Technical/natural sciences

Publication information
Journal: Angewandte Chemie
Volume: 126
Issue number: 46
Oxidation of Bioethanol using Zeolite-Encapsulated Gold Nanoparticles

With the ongoing developments in biomass conversion, the oxidation of bioethanol to acetaldehyde may become a favorable and green alternative to the preparation from ethylene. Here, a simple and effective method to encapsulate gold nanoparticles in zeolite silicalite-1 is reported and their high activity and selectivity for the catalytic gas-phase oxidation of ethanol are demonstrated. The zeolites are modified by a recrystallization process, which creates intraparticle voids and mesopores that facilitate the formation of small and disperse nanoparticles upon simple impregnation. The individual zeolite crystals comprise a broad range of mesopores and contain up to several hundred gold nanoparticles with a diameter of 2-3nm that are distributed inside the zeolites rather than on the outer surface. The encapsulated nanoparticles have good stability and result in 50% conversion of ethanol with 98% selectivity toward acetaldehyde at 200 degrees C, which (under the given reaction conditions) corresponds to 606 mol acetaldehyde/mol Au.hour⁻¹.

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Center for Electron Nanoscopy, Max-Planck-Institut
Authors: Mielby, J. J. (Intern), Abildstrøm, J. O. (Intern), Wang, F. (Ekstern), Kasama, T. (Intern), Weidenthaler, C. (Ekstern), Kegnæs, S. (Intern)
Number of pages: 4
Pages: 12513-12516
Publication date: 2014
Main Research Area: Technical/natural sciences

Publication information
Journal: ANGEWANDTE CHEMIE-INTERNATIONAL EDITION
Volume: 53
Issue number: 46
ISSN (Print): 1433-7851
Ratings:
BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 10.8 SJR 5.8 SNIP 2.104
Selective Oxidations using Nanostructured Heterogeneous Catalysts

The aim of this thesis is to investigate and develop new efficient methods to oxidise alcohols and amines using heterogeneous catalysts and either O₂ or H₂O₂ as oxidants. From an economic and environmental point of view, these oxidants are ideal, because they are cheap and readily available and because they produce H₂O as the only by-product. Chapter 1 gives a short introduction to basic concepts in heterogeneous catalysis and green chemistry. Furthermore, the chapter gives an overview of the most important strategies to synthesise functional nanostructured materials and
highlights how detailed understanding of size, shape and structure can help in the development of new and more efficient heterogeneous catalysts. The chapter is not intended to give a complete survey, but rather to introduce some of the recent developments in the synthesis of nanostructured heterogeneous catalysts. Finally, the chapter focuses on the use of supported metal catalysts for the selective oxidation of alcohols, which are currently dominated by the platinum group metals. Chapter 2 deals with the most important methods to characterise heterogeneous catalysts, including X-ray powder diffraction, physisorption analysis and electron microscopy. In particular, the chapter gives an introduction to electron tomography, which makes it possible to visualise and analyse the detailed three-dimensional features of nanostructured heterogeneous catalysts. Chapter 3 deals with the surprisingly high catalytic activity of supported gold nanoparticles with particular emphasis on the nature of the active site and the requirements needed to be considered when designing new catalytic systems. Furthermore, the chapter describes some of the most important methods to synthesise small and disperse gold nanoparticles on different supports. Chapter 4 describes a novel method for the two-step synthesis of amides from alcohols and amines using Au/TiO₂ and base as catalysts. In the first step, a methyl ester is obtained by the gold-catalysed aerobic oxidation of the alcohol in methanol. Base is promoting this reaction. In the second step, the amine is added and the methyl ester undergoes base-catalysed aminolysis to give the desired amide. As the same base is used for both reactions, the synthesis could be performed in a convenient one-pot procedure. The oxidative coupling was applied to a number of different alcohols and amines to demonstrate the versatility of the reaction protocol to a broader range of substrates. Chapter 5 describes the investigation of different silver catalysts for the synthesis of imines from alcohols and amines. The reactions were performed at relatively mild conditions (100°C and atmospheric pressure) without any additives or co-catalysts and afforded the desired imines with high selectivity (up to 99%). The highest catalytic activity was obtained with 5 wt% Ag/Al₂O₃ in toluene with air as oxidant, although the reaction also occurred under inert atmosphere by releasing H₂ into the gas-phase. Chapter 6 gives a short introduction to zeolites and the important concept of shape selectivity. Furthermore, the chapter describes the different strategies that can be used to overcome diffusion limitations. Chapter 7 demonstrates that mesoporous titanium silicalite-1 prepared by carbon templating is an efficient catalyst for oxidation of pyridines to pyridine N-oxides using aqueous H₂O₂ as oxidant. The chapter begins with an introduction to N-oxides and an outline of recent development in the synthesis of ordered titanosilicates with focus on the efforts to overcome diffusion limitations. Chapter 8 describes how the continuing technological developments in biomass processing have made bioethanol a promising platform molecule for the production of a variety of value-added chemicals. Furthermore, the chapter describes a simple and effective method to encapsulate gold nanoparticles into a MFI zeolite and demonstrate their remarkable stability, catalytic activity and selectivity for the gas-phase oxidation of bioethanol to acetaldehyde, which may become a favourable and green alternative to the ethylene route.

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Authors: Mielby, J. J. (Intern), Kegnæs, S. (Intern), Riisager, A. (Intern)
Number of pages: 188
Publication date: 2014

Silver nanoparticles supported on alumina—a highly efficient and selective nanocatalyst for imine reduction
Silver nanoparticles supported on alumina were prepared and tested in the catalytic reduction of various imines to primary and secondary amines and were shown to be exceptionally active and chemoselective. Furthermore, the catalytic activity of the prepared nanocatalyst was also tested in the synthesis of secondary amines from primary amines in a tandem reaction protocol (oxidation–imination–reduction) using air and molecular hydrogen as oxidizing and reducing agents, respectively. The reported synthesis is performed under mild reaction conditions, which complies with the demands of modern organic synthesis. Due to the mild reaction conditions and high conversion as well as high selectivity, we consider that the utilization of silver nanoparticles supported on alumina represents an attractive and environmentally friendly alternative to the current synthesis of N-alkyl amines.

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Authors: Poreddy, R. (Intern), Garcia-Suarez, E. J. (Intern), Riisager, A. (Intern), Kegnæs, S. (Intern)
Pages: 4255–4259
Publication date: 2014
Main Research Area: Technical/natural sciences

Publication information
Catalytic Performance of Zeolite-Supported Vanadia in the Aerobic Oxidation of 5-hydroxymethylfurfural to 2,5-diformylfuran

The catalytic performance of zeolite-supported vanadia catalysts was examined for the aerobic oxidation of 5-hydroxymethylfurfural (HMF) to 2,5-diformylfuran (DFF) in organic solvents such as N,N-dimethylformamide (DMF), methyl isobutyl ketone, toluene, trifluorotoluene and DMSO. Catalysts based on the four different zeolite supports H-beta, H-Y, H-mordenite, and H-ZSM-5 with 1–10 wt% vanadia loading were prepared and characterized by nitrogen physisorption, X-ray powder diffraction, scanning electron microscopy, ammonia temperature-programmed desorption, Raman spectroscopy and UV/Vis spectrophotometry. The H-beta zeolite catalysts were found to contain highly dispersed vanadium oxide species at all loadings, and provided the highest reaction selectivity towards DFF and the lowest metal leaching of the examined systems. In particular, 1 wt % V₂O₅/H-beta was found to be a stable, recyclable, and non-leaching catalyst for the production of DFF under mild conditions in DMF as solvent, although with low DFF yield. To increase the yield, oxidation of HMF at elevated pressures was also investigated with this catalyst. Under optimized conditions, a reaction selectivity towards DFF of >99 % at 84 % HMF conversion was obtained, albeit with some contribution from lixiviated species to the total catalyst activity.

General Information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Pages: 284-293
Publication date: 2013
Main Research Area: Technical/natural sciences

Publication Information
Journal: ChemCatChem
Volume: 5
Issue number: 1
ISSN (Print): 1867-3880
Ratings:
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.33 SJR 1.636 SNIP 0.932
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.751 SNIP 1 CiteScore 4.57
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.88 SNIP 1.102 CiteScore 4.52
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 2.167 SNIP 1.06 CiteScore 4.82
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Scopus rating (2012): SJR 2.375 SNIP 1.142 CiteScore 4.58
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
Scopus rating (2011): SJR 2.238 SNIP 1.056 CiteScore 4.3
ISI indexed (2011): ISI indexed no
Scopus rating (2010): SJR 1.664 SNIP 0.926
Epoxidation of Alkenes with Aqueous Hydrogen Peroxide and Quaternary Ammonium Bicarbonate Catalysts

A range of solid and liquid catalysts containing bicarbonate anions were synthesised and tested for the epoxidation of alkenes with aqueous hydrogen peroxide. The combination of bicarbonate anions and quaternary ammonium cations opens up for new catalytic systems that can help to overcome challenges with catalyst separation and reuse.

General information

State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Authors: Mielby, J. J. (Intern), Kegnæs, S. (Intern)
Pages: 1162-1165
Publication date: 2013
Main Research Area: Technical/natural sciences

Publication information

Journal: Catalysis Letters
Volume: 143
Issue number: 11
ISSN (Print): 1011-372x
Ratings:
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.39 SJR 0.733 SNIP 0.768
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.757 SNIP 0.757 CiteScore 2.27
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.895 SNIP 0.937 CiteScore 2.56
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.894 SNIP 0.935 CiteScore 2.45
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.016 SNIP 0.988 CiteScore 2.35
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.07 SNIP 0.993 CiteScore 2.47
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.07 SNIP 0.792
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.996 SNIP 0.887
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.113 SNIP 0.858
Mechanistic investigation of the one-pot formation of amides by oxidative coupling of alcohols with amines in methanol

The one-pot formation of amides by oxidative coupling of alcohols and amines via intermediate formation of methyl ester using supported gold and base as catalysts was studied using the Hammett methodology. Determining the relative reactivity of four different para-substituted benzyl alcohol derivatives showed that the first step of the reaction generates a partial positive charge in the benzylic position (i.e. by hydride abstraction), while the second step of the reaction builds up negative charge in the rate determining step. The aminolysis of the methyl ester intermediate was further investigated by means of DFT/B3LYP. The transition state structures and energies were determined for both a concerted and a neutral two-step reaction mechanism. As expected, the base-promoted two-step mechanism was found to be the most energetically favourable and this reaction mechanism was used to construct a theoretical Hammett plot that was in good agreement with the one obtained experimentally.
Separation of Flue Gas Components by SILP (Supported Ionic Liquid-Phase) Absorbers

Reversible absorption of the flue gas components CO₂, NO, NO₂ and SO₂ has been tested for different ionic liquids (ILs) at different temperatures and flue gas compositions where porous, high surface area carriers have been applied as supports for the ionic liquids to obtain Supported Ionic Liquid-Phase (SILP) absorber materials. The use of solid SILP absorbers with selected ILs were found to significantly improve the absorption capacity and sorption dynamics at low flue gas concentration, thus making the applicability of ILs viable in technical, continuous flow processes for flue gas cleaning. The results show that CO₂, NO and SO₂ can be reversible and selective absorbed using different ILs and that Supported Ionic Liquid-Phase (SILP) absorbers are promising materials for industrial flue gas cleaning. Absorption/desorption dynamics can be tuned by temperature, pressure and gas concentration.

© 2012 ECS - The Electrochemical Society
Acetic Acid Formation by Selective Aerobic Oxidation of Aqueous Ethanol over Heterogeneous Ruthenium Catalysts

Heterogeneous catalyst systems comprising ruthenium hydroxide supported on different carrier materials, titania, alumina, ceria, and spinel (MgAl2O4), were applied in selective aerobic oxidation ethanol to form acetic acid, an important bulk chemical and food ingredient. The catalysts were characterized by X-ray powder diffraction (XRPD), transmission electron microscopy (TEM), energy dispersive spectroscopy (EDS), and nitrogen physisorption and utilized in the oxidation of 2.5–50 wt % aqueous ethanol solutions at elevated temperatures and pressures. The effects of Ru metal loading, pretreatment of catalysts, oxidant pressure, reaction temperature, and substrate concentration were investigated. Quantitative yield of acetic acid was obtained with 1.2 wt % Ru(OH)x/CeO2 under optimized conditions (150 °C, 10 bar O2, 12 h of reaction time, 0.23 mol % Ru to substrate).

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Center for Electron Nanoscopy
Authors: Gorbanev, Y. (Intern), Kegnæs, S. (Intern), Hanning, C. W. (Intern), Hansen, T. W. (Intern), Riisager, A. (Intern)
Pages: 604-612
Catalytic conversion of alcohols to fuels and chemicals

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Authors: Mentzel, U. V. (Intern), Mielby, J. J. (Intern), Holm, M. S. (Ekstern), Kegnæs, S. (Intern)
Publication date: 2012
Main Research Area: Technical/natural sciences
Publication: Research - peer-review » Journal article – Annual report year: 2012

Gold Nanoparticle-Catalyzed Formation of Nitrogen-containing Compounds-From Mechanistic Understanding to Synthetic Exploitation
During the last decade, heterogeneous catalysis using gold nanoparticles has gained importance as an efficient method for the oxidation of alcohols and aldehydes. The scope of these reactions has recently been extended to nitrogen-containing compounds, which is a particularly promising substrate class, as nitrogen is ubiquitous in both materials science and biology. It has been shown that gold nanoparticles can overcome many of the frequently encountered difficulties caused by the coordinating properties of nitrogen when using homogenous catalysis. This minireview is meant to serve as an entry point for new researchers in this emerging field and is divided into sections based upon which nitrogen-containing products are synthesized using gold nanoparticles in the critical reaction step.

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry
The increasing need for shifting to renewable feedstocks in the chemical industry has driven research toward using green aerobic, selective oxidation reactions to produce bulk chemicals. Here, we report the use of a ruthenium mixed oxide/hydroxide (RuOx) on different support materials for the selective aerobic oxidation of ethanol to acetic acid. The RuOx was deposited onto different oxide supports using a new gas-phase reaction, which in all cases resulted in homogeneous nanoparticulate films. The RuOx particle size ranged from 0.3 to 1.5 nm. The catalytic activity was evaluated on TiO2, Mg6Al2(CO3)(OH)16·4(H2O), MgAl2O4, Na2Ti6O13 nanotubes, ZnO,γ-Al2O3, WO3, CeO2, and Ce0.5Zr0.5O2 supports. The CeO2 supported RuOx had the highest activity, and selectivity toward acetic acid, of all the materials when normalized with respect to Ru-loading. This high activity was independent of the surface area of the support and the loading of RuOx under the tested conditions. This was attributed to the highly uniform size of the RuOx deposits, demonstrating that the deposition is suitable for producing small nanoparticles at high loadings. To elucidate the reason for the promotional effect of CeO2, Ce0.5Zr0.5O2 was investigated as a high oxygen storage capacity support, however, this did not result in higher catalytic activity. The high activity of CeO2 supports compared to the low activity ZnO appear correlated to the presence of high valence Ru(VI) species analogous to that observed in literature.
Molybdenum sulfides-efficient and viable materials for electro - and photoelectrocatalytic hydrogen evolution
This perspective covers the use of molybdenum disulfide and related compounds, generally termed MoSx, as electro- or photoelectrocatalysts for the hydrogen evolution reaction (HER). State of the art solutions as well as the most illustrative results from the extensive electro- and photoelectrocatalytic literature are given. The research strategies currently employed in the field are outlined and future challenges pointed out. We suggest that the key to optimising the HER activity of MoS2 is divided into (1) increasing the catalytic activity of the active site, (2) increasing the number of active sites of the catalyst, and (3) improving the electrical contact to these sites. These postulations are substantiated by examples from the existing literature and some new results. To demonstrate the electrocatalytic properties of a highly conductive MoS2 hybrid material, we present the HER activity data for multi-wall MoS2 nanotubes on multi-wall carbon nanotubes (MWMoS2@MWCNTs). This exemplifies the typical data collected for the electrochemical HER. In addition, it demonstrates that the origin of the activity is closely related to the amount of edges in the layered MoS2. The photoelectrocatalytic HER is also discussed, based on examples from literature, with an emphasis on the use of MoSx as either (1) the co-catalyst providing the HER activity for a semiconductor, e. g. Mo3S4+ on Si or (2) MoS2 as the semiconductor with an intrinsic HER activity. Finally, suggestions for future catalyst designs are given.

General information
State: Published
Organisations: Department of Physics, Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Experimental Surface and Nanomaterials Physics
Authors: Laursen, A. B. (Intern), Kegnæs, S. (Intern), Dahl, S. (Intern), Chorkendorff, I. (Intern)
Pages: 5577-5591
Publication date: 2012
Main Research Area: Technical/natural sciences

Publication information
Journal: Energy & Environmental Science
Volume: 5
Issue number: 2
ISSN (Print): 1754-5692
Ratings:
BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 10.027 SNIP 4.275 CiteScore 23.85
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 7.792 SNIP 4.034 CiteScore 19.28
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 6.02 SNIP 3.011 CiteScore 14.81
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 5.86 SNIP 2.594 CiteScore 11.84
Nanostructured MoS2 for electrocatalytic watersplitting

General information
State: Published
Organisations: Department of Physics, Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Experimental Surface and Nanomaterials Physics
Authors: Laursen, A. B. (Intern), Kegnæs, S. (Intern), Chorkendorff, I. (Intern), Dahl, S. (Intern)
Publication date: 2012
Main Research Area: Technical/natural sciences
Publication: Research - peer-review » Journal article – Annual report year: 2012

One-pot synthesis of amides by aerobic oxidative coupling of alcohols or aldehydes with amines using supported gold and base as catalysts

Synthesis of amides by aerobic oxidative coupling of alcohols or aldehydes with amines via intermediate formation of methyl esters is highly efficient and selective when using a catalytic system comprised of supported gold nanoparticles and added base in methanol.

General information
State: Published
Organisations: Centre for Catalysis and Sustainable Chemistry, Department of Chemistry, Organic Chemistry
Authors: Kegnæs, S. (Intern), Mielby, J. J. (Intern), Mentzel, U. V. (Intern), Jensen, T. (Intern), Fristrup, P. (Intern), Riisager, A. (Intern)
Pages: 2427-2429
Publication date: 2012
Main Research Area: Technical/natural sciences
Publication information
Journal: Chemical Communications
Volume: 48
Issue number: 18
ISSN (Print): 1359-7345
Ratings:
BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 6.06 SJR 2.506 SNIP 1.159
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 2.664 SNIP 1.314 CiteScore 6.7
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.701 SNIP 1.446 CiteScore 6.83
Separation of flue gas components by ionic liquids: Fundamental chemistry and industrial application

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Publication date: 2012
Event: Abstract from Pacific Rim Meeting on Electrochemical and Solid-State Science, Honolulu, United States.
Aerobic Oxidation Reactions with Highly Selective Gold Nanoparticle Catalysts

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Authors: Mielby, J. J. (Intern), Kegnæs, S. (Intern), Riisager, A. (Intern)
Publication date: 2011
Event: Abstract from The 22nd North American Catalysis Society Meeting, Detroit, United States.
Main Research Area: Technical/natural sciences
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2011

Alternative Flue Gas Cleaning: Selective Gas Absorption by Ionic Liquids and by Supported Ionic Liquid-Phase (SILP) Absorbers

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Authors: Shunmugavel, S. (Intern), Kegnæs, S. (Intern), Due-Hansen, J. (Intern), Abildstrøm, J. O. (Intern), Riisager, A. (Intern), Fehrmann, R. (Intern)
Publication date: 2011
Main Research Area: Technical/natural sciences
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2011

Effect of Support in Heterogeneous Ruthenium Catalysts Used for the Selective Aerobic Oxidation of HMF in Water

Heterogeneous ruthenium-based catalysts were applied in the selective, aerobic oxidation of 5-hydroxymethylfurfural, a versatile biomass-derived chemical, to form 2,5-furandicarboxylic acid. The oxidation reactions were performed in water with dioxygen as the oxidant at different pressures without added base. Catalysts were prepared by depositing catalytically active Ru(OH)x species on a number of different supports, such as titanium-, aluminum-, cerium-, zirconium-, magnesium- and lanthanum oxides, magnetite, spinel, hydrotalcite and hydroxyapatite. All the catalysts were found to be active in the oxidation reactions, and the choice of support was demonstrated to be important for the catalytic performance.

General information
State: Published
Organisations: Centre for Catalysis and Sustainable Chemistry, Department of Chemistry
Authors: Gorbanev, Y. (Intern), Kegnæs, S. (Intern), Riisager, A. (Intern)
Pages: 1318-1324
Publication date: 2011
Main Research Area: Technical/natural sciences
Publication information
Journal: Topics in Catalysis
Volume: 54
Issue number: 16-18
ISSN (Print): 1022-5528
Ratings:
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.974 SNIP 0.878 CiteScore 2.55
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.945 SNIP 0.789 CiteScore 2.41
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.989 SNIP 0.862 CiteScore 2.29
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Ionic Liquid Gas Absorption of Pollutants in Flue Gases

General information

State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Authors: Due-Hansen, J. (Intern), Kegnæs, S. (Intern), Godiksen, S. (Ekstern), Riisager, A. (Intern), Fehrmann, R. (Intern)
Publication date: 2011
Main Research Area: Technical/natural sciences

Magnesium and nickel(II) furan-2,5-dicarboxylate

The salts hexaaquamagnesium furan-2,5-dicarboxylate, [Mg(H2O)(6)](C6H2O5), (I), and hexaaquanickel furan-2,5-dicarboxylate, [Ni(H2O)(6)](C6H2O5), (II), provide the first crystallographic characterization of the furan-2,5-dicarboxylate dianion. Both structures exhibit extensive three-dimensional hydrogen-bonding networks between the octahedral
coordinated hexaaquametal(II) ions and the dicarboxylate anions. Although the two structures are not isomorphous, they contain essentially identical two-dimensional slabs. The distinction between the structures is that these slabs are related by translation in (II), whereas adjacent slabs in (I) are reflected relative to each other by the action of a glide plane. The reflection occurs so that the local contacts between slabs are not changed, and thus the hydrogen-bond networks are identical except for the orientation of the water molecules at the interface between slabs.

**General information**

State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, University of Copenhagen
Authors: Schau-Magnussen, M. (Ekstern), Gorbanev, Y. (Intern), Kegnaes, S. (Intern), Riisager, A. (Intern)
Pages: M327-M330
Publication date: 2011
Main Research Area: Technical/natural sciences

**Publication information**

Journal: Acta Crystallographica. Section C: Crystal Structure Communications
Volume: 67
ISSN (Print): 0108-2701
Ratings:
- BFI (2017): BFI-level 1
- Web of Science (2017): Indexed Yes
- BFI (2016): BFI-level 1
- Scopus rating (2016): SJR 0.97 SNIP 1.523 CiteScore 3.17
- BFI (2015): BFI-level 1
- Scopus rating (2015): SJR 0.242 SNIP 0.27 CiteScore 0.57
- BFI (2014): BFI-level 1
- Scopus rating (2014): SJR 0.198 SNIP 0.335
- BFI (2013): BFI-level 1
- Scopus rating (2013): SJR 0.293 SNIP 0.397
- ISI indexed (2013): ISI indexed yes
- BFI (2012): BFI-level 1
- Scopus rating (2012): SJR 0.262 SNIP 0.388
- ISI indexed (2012): ISI indexed yes
- BFI (2011): BFI-level 1
- Scopus rating (2011): SJR 0.271 SNIP 0.396
- ISI indexed (2011): ISI indexed yes
- Web of Science (2011): Indexed yes
- BFI (2010): BFI-level 1
- Scopus rating (2010): SJR 0.363 SNIP 0.396
- BFI (2009): BFI-level 1
- Scopus rating (2009): SJR 0.267 SNIP 0.442
- BFI (2008): BFI-level 1
- Scopus rating (2008): SJR 0.409 SNIP 0.411
- Scopus rating (2007): SJR 0.397 SNIP 0.804
- Scopus rating (2006): SJR 0.402 SNIP 0.898
- Web of Science (2006): Indexed yes
- Scopus rating (2005): SJR 0.377 SNIP 0.425
- Web of Science (2005): Indexed yes
- Scopus rating (2004): SJR 0.37 SNIP 0.517
- Scopus rating (2003): SJR 0.337 SNIP 0.508
- Web of Science (2003): Indexed yes
- Scopus rating (2002): SJR 0.372 SNIP 0.531
- Scopus rating (2001): SJR 0.374 SNIP 0.499
- Scopus rating (2000): SJR 0.365 SNIP 0.501
- Scopus rating (1999): SJR 0.414 SNIP 0.651

Original language: English
Electronic versions:
One-pot synthesis of amides by aerobic oxidative coupling of alcohols and amines using supported gold and base as catalysts

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Authors: Mielby, J. J. (Intern), Kegnæs, S. (Intern), Riisager, A. (Intern)
Publication date: 2011
Event: Abstract from 10th EuropaCat Congress, Glasgow, United Kingdom.
Main Research Area: Technical/natural sciences
Publication: Research - peer-review › Journal article – Annual report year: 2011

Selective Aerobic Oxidation of 5-Hydroxymethylfurfural in Water Over Solid Ruthenium Hydroxide Catalysts with Magnesium-Based Supports

Solid catalyst systems comprised of ruthenium hydroxide supported on magnesium-based carrier materials (spinel, magnesium oxide and hydrotalcite) were investigated for the selective, aqueous aerobic oxidation of the biomass-derived chemical 5-hydroxymethylfurfural into 2,5-furandicarboxylic acid (FDA), a possible plastics precursor. The novel catalyst systems were characterized by nitrogen physisorption, XRPD, TEM and EDS analysis, and applied for the oxidation with no added base at moderate to high pressures of dioxygen and elevated temperatures. The effects of support, temperature and oxidant pressure were studied and optimized to allow a quantitative yield of FDA to be obtained.

General information
State: Published
Organisations: Centre for Catalysis and Sustainable Chemistry, Department of Chemistry
Authors: Gorbanev, Y. (Intern), Kegnæs, S. (Intern), Riisager, A. (Intern)
Pages: 1752-1760
Publication date: 2011
Main Research Area: Technical/natural sciences
Publication information
Journal: Catalysis Letters
Volume: 141
Issue number: 12
ISSN (Print): 1011-372X
Ratings:
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.39 SJR 0.733 SNIP 0.768
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.757 SNIP 0.757 CiteScore 2.27
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.895 SNIP 0.937 CiteScore 2.56
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.894 SNIP 0.935 CiteScore 2.45
ISI indexed (2013): ISI indexed yes
Size-Selective Oxidation of Aldehydes with Zeolite Encapsulated Gold Nanoparticles

Here, we report a synthesis and catalytic study of hybrid materials comprised of 1–3 nm sinter-stable Au nanoparticles in MFI-type zeolites. An optional post-treatment in aqua regia effectively removes Au from the external surfaces. The size-selective aerobic aldehyde oxidation verifies that the active Au is accessible only through the zeolite micropores.

General information
State: Published
Organisations: Centre for Catalysis and Sustainable Chemistry, Department of Chemistry, Experimental Surface and Nanomaterials Physics, Department of Physics, Lindoe Offshore Renewables Center
Authors: Højholt, K. T. (Intern), Laursen, A. B. (Intern), Kegnæs, S. (Intern), Christensen, C. H. (Ekstern)
Pages: 1026-1033
Publication date: 2011
Main Research Area: Technical/natural sciences

Publication information
Formation of imines by selective gold-catalysed aerobic oxidative coupling of alcohols and amines under ambient conditions

The formation of imines by aerobic oxidative coupling of mixtures of alcohols and amines was studied using gold nanoparticles supported on titanium dioxide, TiO₂, as a heterogeneous catalyst. The reactions were performed at ambient conditions (room temperature and atmospheric pressure) and occurred with excellent selectivity (above 98%) at moderate conversion under optimized conditions. The effect of catalytic amounts of different bases was studied, along with reaction temperature and time. Utilisation of a selective catalyst system that uses dioxygen as an oxidant and only produces water as by-product represents a new green reaction protocol for imine formation.

General information

State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Administration, Department of Chemical and Biochemical Engineering
Authors: Kegnæs, S. (Intern), Mielby, J. J. (Intern), Mentzel, U. V. (Intern), Christensen, C. H. (Intern), Riisager, A. (Intern)
Pages: 1437-1441
Publication date: 2010
Main Research Area: Technical/natural sciences

Publication information

Journal: Green Chemistry
Volume: 12
ISSN (Print): 1463-9262
Ratings:
BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): SJR 2.564 SNIP 2.019 CiteScore 8.86
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 2.477 SNIP 1.901 CiteScore 8.21
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.398 SNIP 2.007 CiteScore 8.05
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.266 SNIP 1.815 CiteScore 7.44
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 2.439 SNIP 1.709 CiteScore 6.64
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 2.363 SNIP 1.697 CiteScore 6.46
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 2.152 SNIP 1.655
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.101 SNIP 1.791
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.984 SNIP 1.543
Web of Science (2008): Indexed yes
Imine formation by benign oxidative coupling of alcohols and amines using supported gold nanoparticles as catalyst

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Authors: Kegnæs, S. (Intern), Mielby, J. J. (Intern), Mentzel, U. V. (Intern), Riisager, A. (Intern)
Publication date: 2010
Event: Abstract from 14th Nordic Symposium on Catalysis, Helsingør, Denmark.
Main Research Area: Technical/natural sciences

Ionic liquid gas absorption of NOx, COx and SOx, Ionic Liquids in Sustainable Energy and Fuels

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Authors: Shunmugavel, S. (Intern), Due-Hansen, J. (Intern), Kegnæs, S. (Intern), Grétarsdóttir, T. (Ekstern), Riisager, A. (Intern), Fehrmann, R. (Intern)
Publication date: 2010
Main Research Area: Technical/natural sciences

Oxidation with environmentally benign heterogeneous metal catalysts

General information
State: Published
Organisations: Sustainable and Green Chemistry, Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Authors: Eyjolfsdottir, E. (Intern), Kegnæs, S. (Intern), Riisager, A. (Intern)
Publication date: 2010
Event: Poster session presented at 14th Nordic Symposium on Catalysis, Helsingør, Denmark.
Main Research Area: Technical/natural sciences
Electronic versions:
poster_nsc2010-final.pdf
Source: orbit
Source-ID: 278083
Publication: Research › Poster – Annual report year: 2010
Renewable building block for plastic industry: Gold-catalyzed oxidation of HMF to FDA in water

General information
State: Published
Organisations: Department of Chemistry, Sustainable and Green Chemistry, Centre for Catalysis and Sustainable Chemistry
Authors: Eyjolfsdottir, E. (Intern), Kegnæs, S. (Intern), Riisager, A. (Intern)
Publication date: 2010
Event: Abstract from 14th Nordic Symposium on Catalysis, Helsingør, Denmark.
Main Research Area: Technical/natural sciences
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2010

Selective amide and imine formation by benign oxidation of alcohols and amines using supported gold nanoparticles as catalyst

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Authors: Kegnæs, S. (Intern), Mielby, J. J. (Intern), Mentzel, U. V. (Intern), Riisager, A. (Intern)
Publication date: 2010
Main Research Area: Technical/natural sciences
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2010

Selective flue gas cleaning with ionic liquids

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, X-ray Crystallography, Energy and Materials
Authors: Kegnæs, S. (Intern), Due-Hansen, J. (Intern), Harris, P. (Intern), Berg, R. W. (Intern), Riisager, A. (Intern), Fehrmann, R. (Intern)
Publication date: 2010
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 271711
Publication: Research - peer-review › Poster – Annual report year: 2010
Selective flue gas cleaning with ionic liquids

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Authors: Kegnæs, S. (Intern), Due-Hansen, J. (Intern), Berg, R. W. (Intern), Riisager, A. (Intern), Fehrmann, R. (Intern)
Publication date: 2010
Main Research Area: Technical/natural sciences
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2010

Selective gas absorption by ionic liquids
Reversible absorption performance for the flue gas components CO2, NO and SO2 has been tested for several different ionic liquids (ILs) at different temperatures and flue gas compositions. Furthermore, different porous, high surface area carriers have been applied as supports for the ionic liquids to obtain Supported Ionic Liquid-Phase (SILP) absorber materials. The use of solid SILP absorbers with selected ILs were found to significantly improve the absorption capacity and sorption dynamics at low flue gas concentration, thus making the applicability of ILs viable in technical, continuous flow processes for flue gas cleaning. The results show that CO2, NO and SO2 can be reversible and selective absorbed using different ILs and that Supported Ionic Liquid-Phase (SILP) absorbers are promising materials for industrial flue gas cleaning. Absorption/desorption dynamics can be tuned by temperatures, pressures and gas concentrations. © The Electrochemical Society.

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Technical University of Denmark
Authors: Shunmugavel, S. (Intern), Kegnæs, S. (Intern), Due-Hansen, J. (Intern), Gretasdottir, T. (Ekstern), Riisager, A. (Intern), Fehrmann, R. (Intern)
Pages: 117-126
Publication date: 2010
Main Research Area: Technical/natural sciences

Publication information
Journal: ECS Transactions
Volume: 33
Issue number: 7
ISSN (Print): 1938-5862
Ratings:
BFI (2017): BFI-level 1
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 0.4 SJR 0.231 SNIP 0.246
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.214 SNIP 0.257 CiteScore 0.36
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.214 SNIP 0.246 CiteScore 0.36
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.192 SNIP 0.237 CiteScore 0.27
ISI indexed (2013): ISI indexed no
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.24 SNIP 0.263 CiteScore 0.29
ISI indexed (2012): ISI indexed no
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.262 SNIP 0.284 CiteScore 0.36
ISI indexed (2011): ISI indexed no
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.247 SNIP 0.245
BFI (2009): BFI-level 1
Selective gold-catalysed aerobic oxidations under ambient conditions

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Authors: Kegnæs, S. (Intern), Mentzel, U. V. (Intern), Mielby, J. J. (Intern), Christensen, C. H. (Intern), Riisager, A. (Intern)
Publication date: 2010
Event: Abstract from 14th Nordic Symposium on Catalysis, Helsingør, Denmark.
Main Research Area: Technical/natural sciences
Publication: Research - peer-review › Conference article – Annual report year: 2010

Size-selective aerobic oxidation by sinter stable gold nanoparticles embedded in zeolite crystals

General information
State: Published
Organisations: Department of Physics, Department of Energy Conversion and Storage, Imaging and Structural Analysis, Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Authors: Laursen, A. B. (Intern), Højholt, K. T. (Ekstern), Simonsen, S. B. (Intern), Lundegaard, L. F. (Ekstern), Helveg, S. (Ekstern), Kegnæs, S. (Intern), Egeblad, K. (Intern), Christensen, C. H. (Intern)
Publication date: 2010
Event: Abstract from 14th Nordic Symposium on Catalysis, Helsingør, Denmark.
Main Research Area: Technical/natural sciences
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2010

Size-selective Oxidation with Au nanoparticles embedded in Zeolite Crystals

General information
State: Published
Organisations: Department of Physics, Department of Energy Conversion and Storage, Imaging and Structural Analysis, Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Publication date: 2010
Event: Abstract from IZC16 & IMMS7 Engineering of new micro- and meso-structured materials, Sorrento, Italy.
Main Research Area: Technical/natural sciences
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2010

Substrate Size-Selective Catalysis with Zeolite-Encapsulated Gold Nanoparticles
The Dark Crystal: A hybrid material is reported that is comprised of 1-2 nm sized gold nanoparticles, accessible only through zeolite micro pores in a silicalite-1 crystal, as shown by three-dimensional TEM tomography (see picture). Calcination experiments indicate that the embedded nanoparticles are highly stable towards sintering.

General information
State: Published
Organisations: Experimental Surface and Nanomaterials Physics, Department of Physics, Sustainable and Green Chemistry, Department of Chemistry, CHEC Research Centre, Department of Chemical and Biochemical Engineering, Administration
Catalytic Ammonia Decomposition Over Ruthenium Nanoparticles Supported on Nano-Titanates
Nanosized Na2Ti3O7, K2Ti6O13 and Cs2Ti6O13 materials were prepared and used as supports of ruthenium nanoparticles for catalytic ammonia decomposition. It is shown that these catalysts exhibit higher catalytic activity than ruthenium supported on TiO2 nanoparticles promoted with cesium. The difference is attributed to the use of nanostructured materials with incorporated alkali metals in the crystal lattice, which apparently gives a higher effect of the promoter. All samples were characterized by X-ray powder diffraction, transmission electron microscopy and N-2 physisorption measurements. Furthermore, the effect of ruthenium loading on the catalytic decomposition of ammonia was investigated.

General information
State: Published
Organisations: Sustainable and Green Chemistry, Department of Chemistry
Authors: Klerke, A. (Intern), Klitgaard, S. K. (Intern), Fehrmann, R. (Intern)
Pages: 541-546
Publication date: 2009
Main Research Area: Technical/natural sciences

Publication information
Journal: Catalysis Letters
Volume: 130
Issue number: 3-4
ISSN (Print): 1011-372X
Ratings:
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.39 SJR 0.733 SNIP 0.768
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.757 SNIP 0.757 CiteScore 2.27
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.895 SNIP 0.937 CiteScore 2.56
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.894 SNIP 0.935 CiteScore 2.45
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.016 SNIP 0.988 CiteScore 2.35
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.07 SNIP 0.993 CiteScore 2.47
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Conversion of biomass resources into chemicals with integrated catalytic technologies

General information
State: Published
Organisations: Sustainable and Green Chemistry, Department of Chemistry, Center for BioProcess Engineering, Department of Chemical and Biochemical Engineering, BioChemical Engineering
Authors: Riisager, A. (Intern), Søndergaard Hansen, T. (Intern), Ståhlberg, T. (Intern), Kegnæs, S. (Intern), Jensen, J. S. (Intern), Woodley, J. (Intern), Boisen, A. (Intern), Pedersen, S. (Intern)
Publication date: 2009
Event: Abstract from Annual Green Chemistry and Engineering Conference, College Park, MD, USA, .
Main Research Area: Technical/natural sciences
Source: orbit
Source-ID: 257494
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2009

Effect of alloying on carbon formation during ethane dehydrogenation
The structure sensitivity of different transition metals in the hydrogenolysis, dehydrogenation, and coking reactions during ethane conversion has been investigated. The investigated metals, Ni, Ru, Rh, and Pd, are co-impregnated with Ag onto an inactive MgAl2O4 spinel support and tested in the conversion of ethane. A tendency is clear for all catalysts: In the first period of time 100% ethane is converted and roughly half of the carbon is converted into coke and deposited on the catalyst. The other half of the carbon is converted into methane. The active sites in the hydrogenolysis are blocked by coke during the initial period whereafter dehydrogenation of ethane is observed. It has previously been predicted in surface science studies that Ag covers the steps of certain transition metals. Here it is documented that the hydrogenolysis and coking reactions are significantly suppressed by co-impregnation of Ag and Ni. The effect of Ag is limited for Ru since the active sites are self-poisoned by carbon; nor for Rh/spinel is the effect observed, which is possibly due to island formation of Ag on the terraces of the Rh metal. A prolongation of the initial period with hydrogenolysis is observed for Ag-Pd/spinel due to an alloy formation of Ag and Pd at these conditions. From our results it can therefore be
concluded that hydrogenolysis mainly takes place on the steps and kinks of the transition metal particles, dehydrogenation reactions mainly takes place on the terraces, and coking is significantly reduced by covering the steps sites by Ag. This important information can be used in designing new catalysts with improved selectivity and stability.

**General information**

State: Published

Organisations: Department of Physics, Sustainable and Green Chemistry, Department of Chemistry, Experimental Surface and Nanomaterials Physics, Center for Individual Nanoparticle Functionality, Center for Nanoteknologi


Pages: 269-278

Publication date: 2009

Main Research Area: Technical/natural sciences

**Publication information**

Journal: Applied Catalysis A: General

Volume: 358

Issue number: 2

ISSN (Print): 0926-860X

Ratings:

BFI (2017): BFI-level 1

Web of Science (2017): Indexed Yes

BFI (2016): BFI-level 1

Scopus rating (2016): SJR 1.178 SNIP 1.311 CiteScore 4.26

Web of Science (2016): Indexed yes

BFI (2015): BFI-level 1

Scopus rating (2015): SJR 1.203 SNIP 1.394 CiteScore 4.08

Web of Science (2015): Indexed yes

BFI (2014): BFI-level 1

Scopus rating (2014): SJR 1.303 SNIP 1.574 CiteScore 4.04

Web of Science (2014): Indexed yes

BFI (2013): BFI-level 1

Scopus rating (2013): SJR 1.426 SNIP 1.538 CiteScore 4.01

ISI indexed (2013): ISI indexed yes

Web of Science (2013): Indexed yes

BFI (2012): BFI-level 1

Scopus rating (2012): SJR 1.549 SNIP 1.615 CiteScore 3.89

ISI indexed (2012): ISI indexed yes

Web of Science (2012): Indexed yes

BFI (2011): BFI-level 1

Scopus rating (2011): SJR 1.71 SNIP 1.706 CiteScore 4.15

ISI indexed (2011): ISI indexed yes

Web of Science (2011): Indexed yes

BFI (2010): BFI-level 1

Scopus rating (2010): SJR 1.761 SNIP 1.624

Web of Science (2010): Indexed yes

BFI (2009): BFI-level 1

Scopus rating (2009): SJR 1.761 SNIP 1.814

Web of Science (2009): Indexed yes

BFI (2008): BFI-level 2

Scopus rating (2008): SJR 1.853 SNIP 1.763

Web of Science (2008): Indexed yes

Scopus rating (2007): SJR 1.826 SNIP 1.616

Web of Science (2007): Indexed yes

Scopus rating (2006): SJR 1.651 SNIP 1.45

Web of Science (2006): Indexed yes

Scopus rating (2005): SJR 1.639 SNIP 1.605

Web of Science (2005): Indexed yes
The aerobic oxidation of 5-hydroxymethylfurfural, a versatile biomass-derived chemical, is examined in water with a titania-supported gold-nanoparticle catalyst at ambient temperature (30 degrees C). The selectivity of the reaction towards 2,5-furandicarboxylic acid and the intermediate oxidation product 5-hydroxymethyl-2-furancarboxylic acid is found to depend on the amount of added base and the oxygen pressure, suggesting that the reaction proceeds via initial oxidation of the aldehyde moiety followed by oxidation of the hydroxymethyl group of 5-hydroxymethylfurfural. Under optimized reaction conditions, a 71% yield of 2,5-furandicarboxylic acid is obtained at full 5-hydroxymethylfurfural conversion in the presence of excess base.

Gold-Catalyzed Aerobic Oxidation of 5-Hydroxymethylfurfural in Water at Ambient Temperature
The aerobic oxidation of 5-hydroxymethylfurfural, a versatile biomass-derived chemical, is examined in water with a titania-supported gold-nanoparticle catalyst at ambient temperature (30 degrees C). The selectivity of the reaction towards 2,5-furandicarboxylic acid and the intermediate oxidation product 5-hydroxymethyl-2-furancarboxylic acid is found to depend on the amount of added base and the oxygen pressure, suggesting that the reaction proceeds via initial oxidation of the aldehyde moiety followed by oxidation of the hydroxymethyl group of 5-hydroxymethylfurfural. Under optimized reaction conditions, a 71% yield of 2,5-furandicarboxylic acid is obtained at full 5-hydroxymethylfurfural conversion in the presence of excess base.

General information
State: Published
Organisations: Sustainable and Green Chemistry, Department of Chemistry, Center for BioProcess Engineering, Department of Chemical and Biochemical Engineering
Authors: Gorbanev, Y. (Intern), Kegnæs, S. (Intern), Woodley, J. (Intern), Christensen, C. H. (Ekstern), Riisager, A. (Intern)
Pages: 672-675
Publication date: 2009
Main Research Area: Technical/natural sciences

Publication information
Journal: ChemSusChem (Print)
Volume: 2
Issue number: 7
ISSN (Print): 1864-5631
Ratings:
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 6.7 SJR 2.385 SNIP 1.276
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 2.494 SNIP 1.411 CiteScore 7.33
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.863 SNIP 1.663 CiteScore 7.97
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 2.548 SNIP 1.452 CiteScore 6.79
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Scopus rating (2012): SJR 3.046 SNIP 1.563 CiteScore 6.72
ISI indexed (2012): ISI indexed yes
Gold catalyzed aerobic oxidations of alcohols and aldehydes

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Sustainable and Green Chemistry, Department of Chemical and Biochemical Engineering
Authors: Kegnæs, S. (Intern), Mentzel, U. V. (Intern), Jensen, T. (Ekstern), Christensen, C. H. (Intern)
Publication date: 2009
Event: Abstract from 9th European Congress on Catalysis, Salamanca, Spain.
Main Research Area: Technical/natural sciences
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2009

Green aerobic oxidation of HMF

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Authors: Gorbanev, Y. (Intern), Kegnæs, S. (Intern), Boisen, A. (Intern), Riisager, A. (Intern)
Publication date: 2009
Event: Abstract from Annual meeting of the Danish Chemical Society, Odense, Denmark.
Main Research Area: Technical/natural sciences
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2009

Process integration for the conversion of glucose to 2,5-furandicarboxylic acid
The development of biorefineries means that a key feedstock for many new processes will be sugars in various forms, such as glucose or fructose. From these feedstocks a range of chemicals can be synthesized using heterogeneous catalysis, immobilized enzymes, homogeneous catalysts, soluble enzymes, fermentations or combinations thereof. This presents a particularly interesting process integration challenge since the optimal conditions for each conversion step will be considerably different from each other. Furthermore, compared to oil-based refineries the feedstock represents a relatively high proportion of the final product value and therefore yield and selectivity in these steps are of crucial importance. In this paper using the conversion of glucose to 2,5-furandicarboxylic acid and associated products as an example, alternative routes will be compared with respect to achievable selectivity, and achievable yield.
Renewable Chemicals by Sustainable Oxidations using Gold Catalysts

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Authors: Kegnæs, S. (Intern), Gorbanev, Y. (Intern), Taarning, E. (Intern), Christensen, C. H. (Intern)
Publication date: 2009

Host publication information
Title of host publication: Experiments in Green and Sustainable Chemistry
Publisher: Wiley-VCH
Editors: Roesky, H., Kennepohl, D.
Main Research Area: Technical/natural sciences
Publication: Research - peer-review › Book chapter – Annual report year: 2009

Aerobic Oxidation of Alcohols over Gold Catalysts: Role of Acid and Base
Gold nanoparticles are deposited on potassium titanate nanowires and used as heterogeneous catalysts in the aerobic oxidation of benzyl alcohol in methanol to methyl benzoate at ambient conditions. The presence of a catalytic amount of base promotes the reaction and the formation of free benzoic acid during the reaction poisons the catalyst. The activity however, of the catalyst can be restored again by addition of base.

General information
State: Published
Organisations: Sustainable and Green Chemistry, Department of Chemistry, Electrochemistry, Fuel Cells and Solid State Chemistry Division, Risø National Laboratory for Sustainable Energy, Haldor Topsoe AS
Authors: Klitgaard, S. K. (Intern), DeLa Riva, A. T. (Ekstern), Helveg, S. (Ekstern), Werchmeister, R. M. L. (Intern), Christensen, C. H. (Intern)
Pages: 213-217
Publication date: 2008
Main Research Area: Technical/natural sciences

Publication information
Journal: Catalysis Letters
Volume: 126
Issue number: 3-4
ISSN (Print): 1011-372X
Ratings:
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.39 SJR 0.733 SNIP 0.768
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.757 SNIP 0.757 CiteScore 2.27
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.895 SNIP 0.937 CiteScore 2.56
Web of Science (2014): Indexed yes
Aerobic oxidation of aldehydes under ambient conditions using supported gold nanoparticle catalysts

A new, green protocol for producing simple esters by selectively oxidizing an aldehyde dissolved in a primary alcohol has been established, utilising air as the oxidant and supported gold nanoparticles as catalyst. The oxidative esterifications proceed with excellent selectivities at ambient conditions; the reactions can be performed in an open flask and at room temperature. Benzaldehyde is even oxidised at a reasonable rate below -70 degrees C. Acrolein is oxidised to methyl acrylate in high yield using the same protocol.

General information
State: Published
Organisations: Department of Chemistry, Sustainable and Green Chemistry, Work, Technology and Organisation, Department of Management Engineering, Administration, Department of Chemical and Biochemical Engineering
Bio-Petrochemicals

Jo mindre jo bedre: Ultrasmå guldklumper sætter fart på kemien

Gold Catalyzed Aerobic Oxidation of Alcohols and Amines in the Synthesis of Amides, Oximes and Imines

Green Aerobic Oxidation of HMF

Green Oxidations: Synthesis of Amides, Oximes and Imines by Gold Catalyzed Oxidation of Amines and Alcohols
Oxidations of amines with molecular oxygen using bifunctional gold–titania catalysts

Over the past decades it has become clear that supported gold nanoparticles are surprisingly active and selective catalysts for several green oxidation reactions of oxygen-containing hydrocarbons using molecular oxygen as the stoichiometric oxidant. We here report that bifunctional gold–titania catalysts can be employed to facilitate the oxidation of amines into amides with high selectivity. Furthermore, we report that pure titania is in fact itself a catalyst for the oxidation of amines with molecular oxygen under very mild conditions. We demonstrate that these new methodologies open up for two new and environmentally benign routes to caprolactam and cyclohexanone oxime, both of which are precursors for nylon-6.

General information
State: Published
Organisations: Sustainable and Green Chemistry, Department of Chemistry
Pages: 419-423
Publication date: 2008
Main Research Area: Technical/natural sciences

Publication information
Journal: Green Chemistry
Volume: 10
Issue number: 4
ISSN (Print): 1463-9262
Ratings:
BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): SJR 2.564 SNIP 2.019 CiteScore 8.86
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 2.477 SNIP 1.901 CiteScore 8.21
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.398 SNIP 2.007 CiteScore 8.05
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.266 SNIP 1.815 CiteScore 7.44
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 2.439 SNIP 1.709 CiteScore 6.64
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 2.363 SNIP 1.697 CiteScore 6.46
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Titanate Nanowires and Nanotubes in Heterogeneous Catalysis

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Authors: Kegnæs, S. (Intern), Christensen, C. H. (Intern)
Publication date: 2008
Event: Abstract from Kemisk Forenings Årsmøde, Odense, Denmark.
Main Research Area: Technical/natural sciences
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2008

Aerobic Oxidation of Amines using Gold-Titania Catalysts: Two Alternative Green Routes to Nylon Precursors

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Publication date: 2007
Main Research Area: Technical/natural sciences
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2007

A Novel Synthesis of Amides by Gold Catalyzed Aerobic Oxidation of Alcohol and Amine Mixtures

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Authors: Jensen, T. (Ekstern), Kegnæs, S. (Intern), Taarning, E. (Intern), Egeblad, K. (Intern), Christensen, C. H. (Intern)
Publication date: 2007
Main Research Area: Technical/natural sciences
Publication: Research - peer-review › Poster – Annual report year: 2007
Bioethanol: Fuel and Feedstock

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Authors: Jørgensen, B. (Ekstern), Hansen, J. R. (Intern), Falsig, H. (Intern), Egeblad, K. (Intern), Kegnæs, S. (Intern), Christensen, C. H. (Intern)
Publication date: 2007
Event: Poster session presented at From Agenda to Action, Palo Alto, CA, United States.
Main Research Area: Technical/natural sciences
Publication: Research - peer-review › Poster – Annual report year: 2007

Direct Green Synthesis of Amides by Aerobic Oxidation of Alcohol and Amine Mixtures

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Publication date: 2007
Main Research Area: Technical/natural sciences
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2007

Guld og flyvende grise: En opdagelsesrejse ind i nanokemiens verden

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Pages: 24-27
Publication date: 2007
Main Research Area: Technical/natural sciences
Publication information
Journal: LMKF-Bladet
Issue number: 3
ISSN (Print): 0906-0855
Ratings:
ISI indexed (2013): ISI indexed no
ISI indexed (2012): ISI indexed no
ISI indexed (2011): ISI indexed no
Original language: Danish
Publication: Research - peer-review › Journal article – Annual report year: 2007

Mesoporous zeolite and zeotype single crystals synthesized in fluoride media
We report the synthesis and characterization of a series of new mesoporous zeolite and zeotype materials made available by combining new and improved procedures for directly introducing carbon into reaction mixtures with the fluoride route for conventional zeolite synthesis. The mesoporous materials were all prepared by hydrothermal crystallization of gels adsorbed on carbon matrices which were subsequently removed by combustion. The procedures presented here resulted in mesoporous zeolite and zeotypes materials with MFI, MEL, BEA, AFI and CHA framework structures. All samples were characterized by XRPD, SEM, TEM and N-2 physisorption measurements. For the zeolite materials it A as found that mesoporous MFI and MEL structured single crystals could indeed be crystallized from fluoride media using an improved carbon-templating approach. More importantly, it was found that mesoporous BEA-type single crystals could be crystallized from fluoride media by a newly developed procedure presented here. Thus, we here present the only known route to mesoporous BEA-type single crystals, since crystallization of this framework structure from basic media is known to give only nanosized crystals as opposed to mesoporous single crystals. For the zeotype materials it was found that highly crystalline mesoporous materials of AFI and CHA structure types could be synthesized using a newly developed procedure. (c) 2006 Elsevier Inc. All rights reserved.

General information
State: Published
Organisations: Sustainable and Green Chemistry, Department of Chemistry
Self-assembly of C$_{60}$ into highly ordered chain-like structures on HOPG observed at ambient conditions
The observation of chain-like structures of self-assembled C-60 Molecules on HOPG surfaces at room temperature in aerial atmosphere by means of scanning tunneling microscopy is reported. The ca. 2.5 nm center-to-center distance between two fullerene molecules is much larger than in the close-packed layered or film structures Of C-60 usually found on HOPG surfaces. (c) 2007 Elsevier B.V. All rights reserved.
Scopus rating (2008): SJR 1.223 SNIP 0.845
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.136 SNIP 0.86
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.265 SNIP 0.952
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.423 SNIP 1.052
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.51 SNIP 1.078
Scopus rating (2003): SJR 1.605 SNIP 1.053
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 1.454 SNIP 0.978
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 1.719 SNIP 1.018
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 1.744 SNIP 0.96
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 1.876 SNIP 0.977
Original language: English
highly-oriented pyrolytic graphite (HOPG), FULLERENE, C60, SURFACES, SCANNING-TUNNELING-MICROSCOPY,
GRAPHITE, FILMS, nanostructures
DOIs:
10.1016/j.susc.2007.03.022
Source: orbit
Source-ID: 207074
Publication: Research - peer-review › Journal article – Annual report year: 2007

Solceller - et strålende svar på den indlysende udfordring

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Authors: Kegnæs, S. (Intern), Egeblad, K. (Intern), Christensen, C. H. (Intern)
Publication date: 2007

Host publication information
Title of host publication: Nye Kemiske Horisonter
ISBN (Print): 9788791233135
Chapter: 8
Main Research Area: Technical/natural sciences
Publication: Education - peer-review › Book chapter – Annual report year: 2007

Template-directed synthesis of chalcogenide nanostructures

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Authors: Kegnæs, S. (Intern), Egeblad, K. (Intern), Brorson, M. (Ekstern), Hansen, T. (Ekstern), Christensen, C. H. (Intern)
Publication date: 2007

Host publication information
Title of host publication: Abstract from 1stsymposium on Transition metal chalcogenide nanostructures (TMCN07), Rathen, Germany.
Main Research Area: Technical/natural sciences
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2007

Turbostratic boron nitride coated on high-surface area metal oxide templates
Boron nitride coatings on high-surface area MgAl2O4 and Al2O3 have been synthesized and characterized by
transmission electron microscopy and by X-ray powder diffraction. The metal oxide templates were coated with boron
nitride using a simple nitridation in a flow of ammonia starting from ammonium borate adsorbed on MgAl2O4 or gamma-
Al2O3. This procedure resulted in the formation of a turbostratic boron nitride film with a thickness of a few individual BN
layers.
A new method for the synthesis MoS$_2$ nanotubes

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Department of Physics
Authors: Kegnæs, S. (Intern), Egeblad, K. (Intern), Kuhn, L. T. (Intern), Christensen, C. H. (Intern)
Publication date: 2006
Event: Poster session presented at Surface reactivity and Nanocatalysis Summer School, Ebeltoft, Denmark.
Main Research Area: Technical/natural sciences
Publication: Research - peer-review › Poster – Annual report year: 2006

Angular variation of linewidths in single-crystal EPR spectra

General information
State: Published
Organisations: University of Copenhagen
Authors: Klitgaard, S. K. (Intern), Gaalsbøl, F. (Ekstern), Weihe, H. (Ekstern)
Pages: 836-839
Publication date: 2006
Main Research Area: Technical/natural sciences
Publication information
Journal: Spectrochimica Acta Part A: Molecular and Biomolecular Spectroscopy
Volume: 63
ISSN (Print): 1386-1425
Ratings:
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.654 SNIP 0.993 CiteScore 2.47
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.704 SNIP 1.189 CiteScore 2.63
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.626 SNIP 1.208 CiteScore 2.4
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.598 SNIP 1.134 CiteScore 2.2
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.627 SNIP 1.074 CiteScore 2.09
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.608 SNIP 1.172 CiteScore 2.13
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.674 SNIP 0.965
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.557 SNIP 0.938
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.668 SNIP 1.099
Scopus rating (2007): SJR 0.591 SNIP 1.064
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 0.567 SNIP 0.848
Continuous, gas-phase oxidation of bio-ethanol with air using gold catalysts: A green and sustainable process to make acetic acid

Formation of acetic acid by aqueous-phase oxidation of ethanol with air in the presence of a heterogeneous gold catalyst

Wine into vinegar: It is possible to selectively oxidize ethanol into acetic acid in aqueous solution with air as the oxidant and a heterogeneous gold catalyst (see TEM image of supported gold particles) at temperatures of about 423 K and O2 pressures of 0.6 MPa. This reaction proceeds readily in aqueous acidic media with yields of up to 90 % and CO2 as the only major by-product.
heterogeneous catalysis, acetic acid, oxidation, bioethanol, gold
**Formation of Acetic Acid by Aqueous-Phase Oxidation of Ethanol with Air in the Presence of a Heterogeneous Gold Catalyst**

Die selektive Oxidation von Ethanol zu Essigsäure gelingt in wässriger Lösung mit dem Oxidans Luft an einem Gold-Heterogenkatalysator (siehe Bild). Bei 423 K und einem O2-Druck von 0.6 MPa verläuft diese Reaktion glatt in saurer wässriger Lösung in Ausbeuten um 90%. CO2 ist das einzige Nebenprodukt, das in nennenswerten Mengen entsteht.

**General information**
State: Published
Organisations: Department of Chemistry, Organic Chemistry, Centre for Catalysis and Sustainable Chemistry
Pages: 4764–4767
Publication date: 2006
Main Research Area: Technical/natural sciences

**Publication information**
Journal: Angewandte Chemie
Volume: 118
Issue number: 28
ISSN (Print): 0044-8249
Ratings:
BFI (2017): BFI-level 1
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 (2008): Indexed yes
Original language: English
Bioethanol, Essigsäure, Gold, Heterogene Katalyse, Oxidationen

**Gold Catalysed Aqueous-Phase Oxidation of Ethanol by Air**

**General information**
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Authors: Jørgensen, B. (Intern), Hansen, J. R. (Intern), Egeblad, K. (Intern), Kegnæs, S. (Intern), Riisager, A. (Intern), Christensen, C. H. (Intern)
Publication date: 2006
Event: Poster session presented at Surface reactivity and Nanocatalysis Summer School, Ebeltoft, Denmark.
Observation of new chain-like structures of $\text{C}_{60}$ on HOPG at ambient conditions using STM

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Department of Physics
Publication date: 2006
Main Research Area: Technical/natural sciences
Publication: Research - peer-review › Poster – Annual report year: 2006

Simpel metode til selvorganiserings af $\text{C}_{60}$ til en-dimensionelle kædestrukturer

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Department of Physics
Publication date: 2006
Event: Poster session presented at Kemisk Forenings Årsmøde, Odense, Denmark.
Main Research Area: Technical/natural sciences
Publication: Research - peer-review › Poster – Annual report year: 2006

STM imaging of $\text{C}_{60}$ on HOPG at ambient conditions

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Authors: Egeblad, K. (Intern), Kegnæs, S. (Intern), Haahr, L. T. (Intern), Hansen, M. (Ekstern), Christensen, C. H. (Intern)
Publication date: 2006
Event: Poster session presented at Nano-consortium kick-off meeting, Copenhagen, Denmark.
Main Research Area: Technical/natural sciences
Publication: Research - peer-review › Poster – Annual report year: 2006

Størrelsesdirigerede synteser af $\text{MoS}_2$ nanorør

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Department of Physics
Authors: Kegnæs, S. (Intern), Egeblad, K. (Intern), Kuhn, L. T. (Intern), Christensen, C. H. (Intern)
Publication date: 2006
Event: Poster session presented at Kemisk Forenings Årsmøde, Odense, Denmark.
Main Research Area: Technical/natural sciences
Publication: Research - peer-review › Poster – Annual report year: 2006

Surprisingly simple approach for self-assembly of $\text{C}_{60}$ into 1D chain structures

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Department of Physics
Publication date: 2006
Event: Poster session presented at Surface reactivity and Nanocatalysis Summer School, Ebeltoft, Denmark.
Main Research Area: Technical/natural sciences
Publication: Research - peer-review › Poster – Annual report year: 2006
Template-directed growth of MoS_2 nanotubes

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Department of Physics
Authors: Kegnæs, S. (Intern), Egeblad, K. (Intern), Kuhn, L. T. (Intern), Christensen, C. H. (Intern)
Publication date: 2006
Event: Poster session presented at Nano-consortium kick-off meeting, Copenhagen, Denmark.
Main Research Area: Technical/natural sciences
Publication: Research - peer-review › Poster – Annual report year: 2006

Anisotropic Hyperfine Interaction in the Manganese(iii) Hexaaqua Ion

General information
State: Published
Organisations: Paul Scherrer Institut, LCMI-CNRS B.P. 166, University of Copenhagen
Authors: Krivokapic, I. (Ekstern), Noble, C. (Ekstern), Klitgaard, S. K. (Intern), Tregenna-Piggott, P. (Ekstern), Weihe, H. (Ekstern), Barra, A. (Ekstern)
Pages: 3613-3616
Publication date: 2005
Main Research Area: Technical/natural sciences

Publication information
Journal: ANGEWANDTE CHEMIE-INTERNATIONAL EDITION
Volume: 44
Issue number: 23
ISSN (Print): 0570-0833
Ratings:
BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 10.8 SJR 5.8 SNIP 2.104
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 5.958 SNIP 2.235 CiteScore 11.13
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 5.805 SNIP 2.309 CiteScore 10.84
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 5.681 SNIP 2.204 CiteScore 10.7
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 6.362 SNIP 2.338 CiteScore 10.55
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 6.062 SNIP 2.387 CiteScore 10.75
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 5.858 SNIP 2.31
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 5.52 SNIP 2.218
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Trichloro(1,4,7-trimethyl-1,4,7-triazacyclononane)chromium(III)

General information
State: Published
Organisations: University of Copenhagen
Authors: Klitgaard, S. K. (Intern), Magnussen, M. (Ekstern)
Pages: m2616-m2617
Publication date: 2005
Main Research Area: Technical/natural sciences

Publication information
Journal: Acta Crystallographica Section E
Volume: E61
Ratings:
BFI (2017): BFI-level 1
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.128 SNIP 0.055 CiteScore 0.19
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.178 SNIP 0.108 CiteScore 0.17
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.225 SNIP 0.191 CiteScore 0.22
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.225 SNIP 0.214 CiteScore 0.24
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.242 SNIP 0.351 CiteScore 0.35
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.243 SNIP 0.393 CiteScore 0.38
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.184 SNIP 0.231
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.202 SNIP 0.243
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.27 SNIP 0.277
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.299 SNIP 0.724
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 0.281 SNIP 0.679
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.256 SNIP 0.341
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.226 SNIP 0.376
Web of Science (2004): Indexed yes
Original language: English
DOIs:
10.1107/S1600536805037086
Source: orbit
Source-ID: 241143
Publication: Research - peer-review › Journal article – Annual report year: 2005

Projects:

Design of heterogeneous metal catalysts for C-H Functionalization
Department of Chemistry
Period: 01/09/2017 → 31/08/2020
Number of participants: 4
Phd Student:
Bennedsen, Niklas Rosendal (Intern)
Supervisor:
Kramer, Søren (Intern)
Mielby, Jerrik Jørgen (Intern)
Main Supervisor:
Kegnæs, Søren (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Synthesis of heterogeneous base metal catalysis for C-H functionalization
Department of Chemistry
Period: 01/05/2017 → 30/04/2020
Number of participants: 4
Phd Student:
Christensen, David Benjamin (Intern)
Supervisor:
Kramer, Søren (Intern)
Mielby, Jerrik Jørgen (Intern)
Main Supervisor:
Kegnæs, Søren (Intern)

Financing sources
Source: Internal funding (public)
Synthesis of heterogeneous nanoparticle catalysts

Department of Chemistry
Period: 01/03/2017 → 29/02/2020
Number of participants: 3
Phd Student:
Zacho, Simone Louise (Intern)
Supervisor:
Mielby, Jerrik Jørgen (Intern)
Main Supervisor:
Kegnæs, Søren (Intern)

Financing sources
Source: Internal funding (public)

Design of multifunctional heterogeneous catalysts

Department of Chemistry
Period: 01/02/2017 → 31/01/2020
Number of participants: 3
Phd Student:
Rasmussen, Kristoffer Hauberg (Intern)
Supervisor:
Mielby, Jerrik Jørgen (Intern)
Main Supervisor:
Kegnæs, Søren (Intern)

Financing sources
Source: Internal funding (public)

Production of aromatics from light alkanes using metal sulfide catalysts

Department of Chemistry
Period: 01/11/2016 → 31/10/2019
Number of participants: 3
Phd Student:
Goodarzi, Farnoosh (Intern)
Supervisor:
Joensen, Finn Høgni (Ekstern)
Main Supervisor:
Kegnæs, Søren (Intern)

Financing sources
Source: Internal funding (public)

Encapsulation of metal nanoparticles for heterogeneous catalysis

Department of Chemistry
Period: 01/05/2016 → 30/04/2019
Number of participants: 3
Phd Student:
Thumbayil, Rouzana Pulikkal (Intern)
Supervisor:
Mielby, Jerrik Jørgen (Intern)
Main Supervisor:
Kegnæs, Søren (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Eksternt finansieret virksomhed
Project: PhD

**Oxidative catalytic upgrading of carbohydrates and derivatives from biomass**
Department of Chemistry
Period: 01/05/2014 → 31/05/2017
Number of participants: 6
Phd Student:
Modvig, Amalie Elise (Intern)
Supervisor:
Fristrup, Peter (Intern)
Main Supervisor:
Riisager, Anders (Intern)
Examiner:
Kegnæs, Søren (Intern)
Lugue, Rafael (Ekstern)
Nielsen, Ulla Gro (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet
Project: PhD

**Synthesis, characterization and application of novel hierarchical zeolite catalysts**
Department of Chemistry
Period: 01/10/2013 → 31/12/2013
Number of participants: 3
Phd Student:
Korsak, Oxana (Intern)
Supervisor:
Kegnæs, Søren (Intern)
Main Supervisor:
Riisager, Anders (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Samfinansieret - Andet
Project: PhD

**Synthesis, Characterization and Evaluation of Tin-containing Zeolites for Biomass Conversion**
Department of Chemistry
Period: 01/09/2013 → 15/03/2017
Number of participants: 6
Phd Student:
Tolborg, Søren (Intern)
Supervisor:
Sádaba, Irantzu (Intern)
Main Supervisor:
Riisager, Anders (Intern)
Examiner:
Kegnæs, Søren (Intern)
Pedersen, Christian Marcus (Ekstern)
Sels, Bert F. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.
Project: PhD

**Lignin biomass conversion to fuels and chemicals**

Department of Chemistry
Period: 01/06/2013 → 16/06/2016
Number of participants: 7
Phd Student:
Mélián Rodríguez, Mayra (Intern)
Supervisor:
Kegnæs, Søren (Intern)
Shunmugavel, Saravanamurugan (Intern)
Main Supervisor:
Riisager, Anders (Intern)
Examiner:
Duus, Jens Ølgaard (Intern)
Gonzales, Miguel Angel Banares (Ekstern)
Johannsen, Ib (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.

Relations
Publications:
Lignin biomass conversion into chemicals and fuels
Project: PhD

**Design of sintering stable heterogenous nanoparticle catalysts**

Department of Chemistry
Period: 01/05/2013 → 21/06/2017
Number of participants: 6
Phd Student:
Gallas-Hulin, Agata (Intern)
Supervisor:
Riisager, Anders (Intern)
Main Supervisor:
Kegnæs, Søren (Intern)
Examiner:
Mossin, Susanne (Intern)
Rasmussen, Søren Birk (Intern)
Wang, Feng Ryan (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.
Project: PhD

**Design of sintering stable heterogenous nanoparticle catalysts**

Department of Chemistry
Period: 15/03/2013 → 15/02/2017
Number of participants: 6
Phd Student:
Abildstrøm, Jacob Oskar (Intern)
Supervisor:
Riisager, Anders (Intern)
Main Supervisor:
Kegnæs, Søren (Intern)
Examiner:
Harris, Pernille (Intern)
Kolen'ko, Yury V. (Ekstern)
Nedel, Sorin (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.
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

**Catalytic Routes to Renewable Chemicals**
Department of Chemistry
Period: 15/07/2011 → 24/09/2014
Number of participants: 6
Phd Student:
Mielby, Jerrik Jørgen (Intern)
Supervisor:
Kegnæs, Søren (Intern)
Main Supervisor:
Riisager, Anders (Intern)
Examiner:
Ståhl, Kenny (Intern)
Herbst, Konrad (Ekstern)
Stakheev, Alexandr Yu. (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

**Transition metal oxidation catalysis**
Department of Chemistry
Period: 15/04/2010 → 03/02/2014  
Number of participants: 6  
Phd Student: Janstrup, Thomas Rene Hyldekær (Intern)  
Supervisor: Mossin, Susanne (Intern)  
Main Supervisor: Fehrmann, Rasmus (Intern)  
Examiner: Kegnæs, Søren (Intern)  
Bendix, Jesper (Ekstern)  
Morgan, Grace G. (Ekstern)  

Financing sources  
Source: Internal funding (public)  
Name of research programme: 1/3 FUU, 1/3 inst 1/3 Andet  
Project: PhD

Sustainable catalysis with functional ionic liquids  
Department of Chemistry  
Period: 01/11/2009 → 24/06/2013  
Number of participants: 5  
Phd Student: Søndergaard, Helle (Intern)  
Main Supervisor: Riisager, Anders (Intern)  
Examiner: Kegnæs, Søren (Intern)  
Bica, Katharina (Ekstern)  
Vogel, Stefan (Ekstern)  

Financing sources  
Source: Internal funding (public)  
Name of research programme: Institut stipendie (DTU) Samf.  
Project: PhD

Design af Funktionelle Nanomaterialer  
Department of Chemistry  
Period: 15/11/2005 → 01/04/2009  
Number of participants: 6  
Phd Student: Kegnæs, Søren (Intern)  
Supervisor: Christensen, Claus H. (Intern)  
Main Supervisor: Fehrmann, Rasmus (Intern)  
Examiner: Harris, Pernille (Intern)  
Joensen, Finn Hogni (Ekstern)  
Schüth, Ferdi (Ekstern)  

Financing sources  
Source: Internal funding (public)  
Name of research programme: Programbevilling  
Project: PhD