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.
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.
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.
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.

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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
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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.

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Authors: Kegnæs, S. (Intern), Abildstrøm, J. O. (Intern), Mielby, J. J. (Intern)
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Priority number: WO2014EP64430
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WO2015001123A1.pdf
Main Research Area: Technical/natural sciences
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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.

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Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Authors: Kegnæs, S. (Intern), Abildstrøm, J. O. (Intern), Mielby, J. J. (Intern), Gallas-Hulin, A. (Intern)
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Priority date: 05/07/2013
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.

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Center for Electron Nanoscopy, Max-Planck-Institut
Authors: Wang, F. (Ekstern), Mielby, J. J. (Intern), Richter, F. H. (Ekstern), Wang, G. (Ekstern), Prieto, G. (Ekstern), Kasama, T. (Intern), Weidenthaler, C. (Ekstern), Bongard, H. (Ekstern), Kegnæs, S. (Intern), Fuerstner, A. (Ekstern), Schueth, F. (Ekstern)
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Publication date: 2014
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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
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 mesopores 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)
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BFI (2017): BFI-level 1
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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 H2 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.
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**
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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)
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Web of Science (2012): Indexed yes
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BFI (2008): BFI-level 1
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Source: FindIt
Source-ID: 270576955
Publication: Research - peer-review › Journal article – Annual report year: 2014

**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 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
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 over-come 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 outlines of recent development in the synthesis of ordered titanocarbonates 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.
An alternative pathway for production of acetonitrile: ruthenium catalysed aerobic dehydrogenation of ethylamine

The oxidative synthesis of acetonitrile from ethylamine was studied using a supported ruthenium catalyst. The reaction was conducted in both batch and flow processes and high conversions (over 85%) were achieved in both cases. Selectivity of both reactions was improved by optimisation of reaction conditions, achieving over 90% selectivity in the batch process and 80% selectivity in the continuous flow process. The use of a selective solid catalyst that utilises a feedstock that can be derived from biomass, dioxygen as the oxidant and water as the solvent represents a new, green route for the independent and efficient production of acetonitrile.

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Authors: Corker, E. (Intern), Mentzel, U. V. (Intern), Mielby, J. J. (Intern), Riisager, A. (Intern), Fehrmann, R. (Intern)
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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
Scopus rating (2007): SJR 2.129 SNIP 1.554
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.539 SNIP 1.414
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.

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Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Authors: Mielby, J. J. (Intern), Kegnæs, S. (Intern)
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Main Research Area: Technical/natural sciences

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Journal: Catalysis Letters
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Web of Science (2017): Indexed Yes
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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
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.

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Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry
Authors: Mielby, J. J. (Intern), Riisager, A. (Intern), Fristrup, P. (Intern), Kegnæs, S. (Intern)
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Main Research Area: Technical/natural sciences

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Catalytic conversion of alcohols to fuels and chemicals

General information
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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
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Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry
Authors: Mielby, J. (Intern), Kegnaes, S. (Intern), Fristrup, P. (Intern)
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Main Research Area: Technical/natural sciences
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Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
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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
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Scopus rating (2010): SJR 1.664 SNIP 0.926
Web of Science (2010): Indexed yes
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Source-ID: n:oat:DTIC-ART:isi/369678467::19440
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
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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)
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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
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.755 SNIP 1.38 CiteScore 6.73
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 3.09 SNIP 1.347 CiteScore 6.21
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 2.857 SNIP 1.322 CiteScore 5.96
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 2.709 SNIP 1.232
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.588 SNIP 1.252
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 2.791 SNIP 1.236
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 2.851 SNIP 1.237
Web of Science (2007): Indexed yes
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

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 › Conference abstract for conference – Annual report year: 2011

Synergy of boric acid and added salts in the catalytic dehydration of hexoses to 5-hydroxymethylfurfural in water
Boric acid and salts showed a synergistic effect on the dehydration of concentrated aqueous sugar solutions to yield 5-hydroxymethylfurfural.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Authors: Hansen, T. S. (Intern), Mielby, J. J. (Intern), Riisager, A. (Intern)
Pages: 109-114
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
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 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 abstract for conference – Annual report year: 2010

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)
Name of research programme: Fonde
Project: PhD

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)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

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)
Name of research programme: Forskningsrådsfinansiering
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

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