A facile molecularly imprinted polymer-based fluorometric assay for detection of histamine

Histamine is a biogenic amine naturally present in many body cells. It is also a contaminant that is mostly found in spoiled food. The consumption of foods containing high levels of histamine may lead to an allergy-like food poisoning. Analytical methods that can routinely screen histamine are thus urgently needed. In this paper, we developed a facile and cost-effective molecularly imprinted polymer (MIP)-based fluorometric assay to directly quantify histamine. Histamine-specific MIP nanoparticles (nanoMIPs) were synthesized using a modified solid-phase synthesis method. They were then immobilized in the wells of a microplate to bind the histamine in aqueous samples. After binding, o-phthaldialdehyde (OPA) was used to label the bound histamine, which converted the binding events into fluorescent signals. The obtained calibration curve of histamine showed a linear correlation ranging from 1.80 to 44.98 mM with the limit of detection of 1.80 μM. This method was successfully used to detect histamine in spiked dairy milk with a recovery rate of more than 85%.

**General information**

State: Published
Organisations: Department of Micro- and Nanotechnology, NanoChemistry
Authors: Feng, X. (Intern), Ashley, J. (Intern), Zhou, T. (Intern), Halder, A. (Intern), Sun, Y. (Intern)
Pages: 2365-2372
Publication date: 2018
Main Research Area: Technical/natural sciences

**Publication information**

Journal: RSC Advances
Volume: 8
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Ratings:
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
An engineered cell-imprinted substrate directs osteogenic differentiation in stem cells

A cell-imprinted poly(dimethylsiloxane)/hydroxyapatite nanocomposite substrate was fabricated to engage topographical, mechanical, and chemical signals to stimulate and boost stem cell osteogenic differentiation. The physicochemical properties of the fabricated substrates, with nanoscale resolution of osteoblast morphology, were probed using a wide range of techniques including scanning electron microscopy, atomic force microscopy, dynamic mechanical thermal analysis, and water contact angle measurements. The osteogenic differentiation capacity of the cultured stem cells on these substrates was probed by alizarin red staining, ALP activity, osteocalcin measurements, and gene expression analysis. The outcomes revealed that the concurrent roles of the surface patterns and viscoelastic properties of the substrate provide the capability of directing stem cell differentiation toward osteogenic phenotypes. Besides the physical and mechanical effects, we found that the chemical signaling of osteoinductive hydroxyapatite nanoparticles, embedded in the nanocomposite substrates, could further improve and optimize stem cell osteogenic differentiation.

General information
State: Published
Organisations: Department of Chemistry, Amirkabir University of Technology, Pasteur Institute of Iran, Tehran University of Medical Sciences
Authors: Kamguyan, K. (Ekstern), Katbab, A. A. (Ekstern), Mahmoudi, M. (Ekstern), Thormann, E. (Intern), Moghaddam, S. Z. (Intern), Moradi, L. (Ekstern), Bonakdar, S. (Ekstern)
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Publication date: 2018
Main Research Area: Technical/natural sciences

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Journal: Biomaterials Science
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Ratings:
Web of Science (2018): Indexed yes
Scopus rating (2016): CiteScore 4.36 SJR 1.422 SNIP 0.949
Scopus rating (2015): CiteScore 3.84 SJR 1.308 SNIP 0.955
Scopus rating (2014): CiteScore 4.15 SJR 1.201 SNIP 0.89
Original language: English
DOIs: 10.1039/c7bm00733g
Anisotropy enhanced X-ray scattering from solvated transition metal complexes

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

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Department of Chemistry, Department of Electric Power Engineering, University of Iceland, SLAC National Accelerator Laboratory, Technical University of Denmark
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Journal: Journal of Synchrotron Radiation
Volume: 25
Issue number: 2
ISSN (Print): 0909-0495
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BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.86 SJR 1.593 SNIP 1.578
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.161 SNIP 1.396 CiteScore 2.45
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.326 SNIP 1.505 CiteScore 2.58
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.473 SNIP 1.687 CiteScore 2.91
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.558 SNIP 1.273 CiteScore 2.36
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.503 SNIP 1.424 CiteScore 2.45
ISI indexed (2011): ISI indexed yes
A theoretical and experimental benchmark study of core-excited states in nitrogen

vibrational structure of the core-excited states. This makes nitrogen well suited for assessing the accuracy of different electronic structure methods for core excitations. We report high resolution experimental measurements performed at the SOLEIL synchrotron facility. These are compared with theoretical spectra calculated using coupled cluster theory and algebraic diagrammatic construction theory. The coupled cluster singles and doubles with perturbative triples model known as CC3 is shown to accurately reproduce the experimental excitation energies as well as the spacing of the vibrational transitions. The computational results are also shown to be systematically improved within the coupled cluster hierarchy, with the coupled cluster singles, doubles, triples, and quadruples method faithfully reproducing the experimental vibrational structure.

General information
State: Published
Organisations: Department of Chemistry, University of Oslo, Stanford University, Johns Hopkins University, Synchrotron Soleil, Norwegian University of Science and Technology
Authors: Myhre, R. H. (Ekstern), Wolf, T. J. A. (Ekstern), Cheng, L. (Ekstern), Nandi, S. (Ekstern), Coriani, S. (Intern), Gühr, M. (Ekstern), Koch, H. (Ekstern)
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BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.13 SJR 1.073 SNIP 0.755
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.953 SNIP 0.767 CiteScore 1.98
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.386 SNIP 0.989 CiteScore 2.54
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.532 SNIP 1.17 CiteScore 2.95
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.787 SNIP 1.118 CiteScore 2.86
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.805 SNIP 1.207 CiteScore 3.07
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.73 SNIP 1.052
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.003 SNIP 1.104
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 2.189 SNIP 1.12
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 2.163 SNIP 1.108
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 2.176 SNIP 1.266
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 2.27 SNIP 1.359
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 2.229 SNIP 1.369
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 2.121 SNIP 1.322
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 2.256 SNIP 1.341
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 2.381 SNIP 1.362
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 2.576 SNIP 1.423
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 2.133 SNIP 1.419

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Source: FindIt
Source-ID: 2396439440
Bi-functional glycosyltransferases catalyze both extension and termination of pectic galactan oligosaccharides

Pectins are the most complex polysaccharides of the plant cell wall. Based on the number of methylations, acetylations, and glycosidic linkages present in their structures, it is estimated that up to 67 transferase activities are involved in pectin biosynthesis. Pectic galactans constitute a major part of pectin in the form of side chains of rhamnogalacturonan-I. In Arabidopsis, Galactan Synthase 1 (GALS1) catalyzes the addition of galactose units from UDP-Gal to growing β-1,4-galactan chains. However, the mechanisms for obtaining varying degrees of polymerization remain poorly understood. In this study, we show that AtGALS1 is bifunctional, catalyzing both the transfer of galactose from UDP-α-d-Gal and the transfer of an arabinopyranose from UDP-β-l-Arap to galactan chains. The two substrates share a similar structure, but UDP-α-d-Gal is the preferred substrate, with a tenfold higher affinity. Transfer of Araβ to galactan prevents further addition of galactose residues, resulting in a lower degree of polymerization. We show that this dual activity occurs both in vitro and in vivo. The herein described bi-functionality of AtGALS1 may suggest that plants can produce the incredible structural diversity of polysaccharides without a dedicated glycosyltransferase for each glycosidic linkage. This article is protected by copyright. All rights reserved.
Chemical Approach to Biological Safety: Molecular-Level Control of an Integrated Zinc Finger Nuclease

Application of artificial nucleases (ANs) in genome editing is still hindered by their cytotoxicity related to off-target cleavages. This problem can be targeted by regulation of the nuclease domain. Here, we provide an experimental survey of computationally designed integrated zinc finger nucleases, constructed by linking the inactivated catalytic centre and the allosteric activator sequence of the colicin E7 nuclease domain to the two opposite termini of a zinc finger array. DNA specificity and metal binding were confirmed by electrophoretic mobility shift assays, synchrotron radiation circular dichroism spectroscopy, and nano-electrospray ionisation mass spectrometry. In situ intramolecular activation of the nuclease domain was observed, resulting in specific cleavage of DNA with moderate activity. This study represents a new approach to AN design through integrated nucleases consisting of three (regulator, DNA-binding, and nuclease) units, rather than simple chimera. The optimisation of such ANs could lead to safe gene editing enzymes.

General information
State: Published
Organisations: Department of Chemistry, Metalloprotein Chemistry and Engineering, Organic Chemistry, University of Tsukuba, University of Szeged, University of Natural Resources and Life Sciences, MTA-SZTE Bioinorganic Chemistry Research Group
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Journal: Chembiochem
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.64 SJR 1.242 SNIP 0.733
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.255 SNIP 0.748 CiteScore 2.77
Web of Science (2015): Indexed yes
Chemically controlled interfacial nanoparticle assembly into nanoporous gold films for electrochemical applications

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

The use of nucleic acid, DNA and RNA, based strategies to disrupt gene expression as a therapeutic is quickly emerging. Indeed, synthetic oligonucleotides represent a major component of modern gene therapeutics. However, the efficiency and specificity of intracellular uptake for nonmodified oligonucleotides is rather poor. Utilizing RNA based oligonucleotides as therapeutics is even more challenging to deliver, due to extremely fast enzymatic degradation of the RNAs. RNAs get rapidly degraded in vivo and demonstrate large off-target binding events when they can reach and enter the desired target cells. One approach that holds much promise is the utilization of "click chemistry" to conjugate receptor or cell specific targeting molecules directly to the effector oligonucleotides. We discuss here the applications of the breakthrough technology of CuAAC click chemistry and the immense potential in utilizing "click chemistry" in the development of new age targeted oligonucleotide therapeutics.

General information
State: Accepted/In press
Organisations: Department of Chemistry, Organic Chemistry, City of Hope Medical Center, Technical University of Denmark
Authors: Astakhova, K. (Intern), Ray, R. (Ekstern), Taskova, M. (Intern), Uhd, J. (Ekstern), Carstens, A. (Intern), Morris, K. (Ekstern)
Number of pages: 8
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information
Journal: Molecular Pharmaceutics
ISSN (Print): 1543-8384
Cyclopiamines C and D: Epoxide Spiroindolinone Alkaloids from Penicillium sp. CML 3020

Cyclopiamines C (1) and D (2) were isolated from the extract of Penicillium sp. CML 3020, a fungus sourced from an Atlantic Forest soil sample. Their structures and relative configuration were determined by 1D and 2D NMR, HRMS, and UV/vis data analysis. Cyclopiamines C and D belong to a small subset of rare spiroindolinone compounds containing an alkyl nitro group and a 4,5-dihydro-1H-pyrrolo[3,2,1-ij]quinoline-2,6-dione ring system. NMR and MS/HRMS data confirmed the presence of an epoxide unit (C-17-O-C-18) and a hydroxy group at C-5, not observed for their known congeners. Cytotoxic and antimicrobial activities were evaluated.

General information
State: Accepted/In press
Organisations: Department of Biotechnology and Biomedicine, Natural Product Discovery, Department of Chemistry, Organic Chemistry, Fungal Chemodiversity, Universidade Federal de Sao Paulo, German Cancer Research Center (DKFZ), Universidade Federal de Vicosa
Discovery of Intermediates of lacZ β-Galactosidase Catalyzed Hydrolysis Using dDNP NMR

Using dissolution dynamic nuclear polarization, the sensitivity of single scan solution state 13C NMR can be improved up to 4 orders of magnitude. In this study, the enzyme lacZ β-galactosidase from Escherichia coli was subjected to hyperpolarized substrate, and previously unknown reaction intermediates were observed, including a 1,1-linked disaccharide. The enzyme is known for making 1,6-transglycosylation, producing products like allolactose, that are also substrates. To analyze the kinetics, a simple kinetic model was developed and used to determine relative transglycosylation and hydrolysis rates of each of the intermediates, and the novel transglycosylation intermediates were determined as better substrates than the 1,6-linked one, explaining their transient nature. These findings suggest that hydrolysis and transglycosylation might be more complex than previously described.

General information

State: Published
Organisations: Department of Chemistry, Department of Electrical Engineering, Center for Hyperpolarization in Magnetic Resonance, Organic Chemistry
Authors: Kjeldsen, C. (Intern), Ardenkjær-Larsen, J. H. (Intern), Duus, J. Ø. (Intern)
Pages: 3030-3034
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Main Research Area: Technical/natural sciences

Publication information

Journal: Journal of the American Chemical Society
Volume: 140
Issue number: 8
ISSN (Print): 0002-7863
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 13.18 SJR 7.368 SNIP 2.584
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 6.826 SNIP 2.632 CiteScore 12.81
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 6.273 SNIP 2.578 CiteScore 11.92
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 5.953 SNIP 2.455 CiteScore 11.38
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 6.141 SNIP 2.379 CiteScore 10.37
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 5.447 SNIP 2.336 CiteScore 9.94
ISI indexed (2011): ISI indexed yes
Dual Nicotinic Acetylcholine Receptor α4β2 Antagonists/α7 Agonists: Synthesis, Docking Studies, and Pharmacological Evaluation of Tetrahydroisoquinolines and Tetrahydroisoquinolinium Salts

We describe the synthesis of tetrahydroisoquinolines and tetrahydroisoquinolinium salts together with their pharmacological properties at various nicotinic acetylcholine receptors. In general, the compounds were α4β2 nAChR antagonists, with the tetrahydroisoquinolinium salts being more potent than the parent tetrahydroisoquinoline derivatives. The most potent α4β2 antagonist, 6c, exhibited submicromolar binding Ki and functional IC50 values and high selectivity for this receptor over the α4β4 and α3β4 nAChRs. Whereas the (S)-6c enantiomer was essentially inactive at α4β2, (R)-6c was a slightly more potent α4β2 antagonist than the reference β2-nAChR antagonist DHβE. The observation that the α4β2 activity resided exclusively in the (R)-enantiomer was in full agreement with docking studies. Several of tetrahydroisoquinolinium salts also displayed agonist activity at the α7 nAChR. Preliminary in vivo evaluation revealed antidepressant-like effects of both (R)-5c and (R)-6c in the mouse forced swim test, supporting the therapeutic potential of α4β2 nAChR antagonists for this indication.

General information
State: Accepted/In press
Organisations: Center for Nuclear Technologies, The Hevesy Laboratory, Department of Chemistry, University of Copenhagen, Technical University of Denmark
Authors: Crestey, F. (Ekstern), Jensen, A. A. (Ekstern), Soerensen, C. (Intern), Magnus, C. B. (Intern), Andreasen, J. T. (Ekstern), Peters, G. H. (Intern), Kristensen, J. L. (Ekstern)
Number of pages: 11
Publication date: 2018
Main Research Area: Technical/natural sciences
Publication information
Journal: Journal of Medicinal Chemistry
Effects of Alkali and Counter Ions in Sn-Beta Catalyzed Carbohydrate Conversion

Alkali ions have been shown to strongly influence the catalytic behavior of stannosilicates in the conversion of carbohydrates. An effect of having alkali ions present is a pronounced increase in selectivity towards methyl lactate. Mechanistic details of this effect have remained obscure and are herein addressed experimentally through kinetic experiments and isotope tracking. Alkali ions have a differential effect in competing reaction pathways: they promote the...
rate of carbon-carbon bond breakage of carbohydrate substrates, but decrease the rates of competing dehydration pathways. Further addition of alkali inhibits activity of Sn-Beta in all major reaction pathways. The alkali effects on product distributions and on rates of product formation are similar, thus pointing to a kinetic reaction control and to irreversible reaction steps in the main pathways. Additionally, an effect of the accompanying basic anions is shown, supposedly facilitating the cation exchange and eliciting a different concentration-dependent effect than neutral alkali salts.

**General information**

State: Accepted/In press
Organisations: Department of Chemistry, Organic Chemistry, Haldor Topsoe AS
Authors: Elliot, S. G. (Intern), Tolborg, S. (Ekstern), Madsen, R. (Intern), Taarning, E. (Ekstern), Meier, S. (Intern)
Number of pages: 6
Publication date: 2018
Main Research Area: Technical/natural sciences

**Publication information**

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ISSN (Print): 1864-5631
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BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
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
Scopus rating (2011): SJR 2.767 SNIP 1.504 CiteScore 5.53
ISI indexed (2011): ISI indexed no
Web of Science (2011): Indexed yes
Scopus rating (2010): SJR 1.945 SNIP 1.134
Web of Science (2010): Indexed yes
Scopus rating (2009): SJR 0.973 SNIP 0.72
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.291 SNIP 0.48
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.273 SNIP 0.495
Scopus rating (2006): SJR 0.243 SNIP 0.372
Scopus rating (2005): SJR 0.195 SNIP 0.285
Scopus rating (2004): SJR 0.214 SNIP 0.276
Scopus rating (2003): SJR 0.276 SNIP 0.419
Scopus rating (2002): SJR 0.312 SNIP 0.586
Scopus rating (2001): SJR 0.292 SNIP 0.496
Scopus rating (2000): SJR 0.422 SNIP 0.556
Scopus rating (1999): SJR 0.511 SNIP 0.708
Original language: English

DOIs:
Elasticity and electrical resistivity of chalk and greensand during water flooding with selective ions

Water flooding with selective ions has in some cases lead to increased oil recovery. We investigate the physical processes on a pore scale that are responsible for changes in petrophysical and mechanical properties of four oil-bearing chalk and four oil-bearing greensand samples caused by flooding with brines containing varying amounts of dissolved NaCl, Na₂SO₄, MgCl₂ and MgSO₄. Ultrasonic P-wave velocity and AC resistivity measurements were performed prior to, during and after flow through experiments in order to identify and quantify the processes related to water flooding with selective ions. Low field Nuclear Magnetic Resonance (NMR) spectrometry measurements were performed at full water saturation, at irreducible water saturation, after aging and after flooding. CT-scanning, X-ray diffraction (XRD), backscatter electron microscopy images (BSEM), mercury injection capillary pressure (MICP) curves and specific surface analysis (BET) reveal the mineralogy and texture of the rock samples before and after the injection. Low field NMR data indicates changes in the pore fluid distribution and wettability of chalk after aging of one of the samples. NMR data for other samples indicate that chalk is water-wet after flooding. Greensand remained mixed wet throughout the experiments. Electrical resistivity data are in agreement with this interpretation. The electrical resistivity data during flooding revealed that the formation brine is not fully replaced by the injected water in both chalk and greensand. Changes in the elasticity of chalk during flooding illustrate the softening effect of magnesium bearing brines as compared to the sodium bearing brines. The stiffness of greensand was not affected by water flooding with selective ions as determined from the elastic wave measurements. Precipitation of fines during flooding of chalk samples is indicated by an increase in specific surface area and a shift in the MICP to lower values but no fines were detected by NMR. No changes were observed for greensand samples.

General information
State: Published
Organisations: Department of Civil Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Ressources Engineering, Department of Chemistry, Section for Geotechnics and Geology, University Savoie Mont Blanc, Politecnico di Torino
Pages: 204–218
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Petroleum Science and Engineering
Volume: 161
ISSN (Print): 0920-4105
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BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.56 SJR 0.764 SNIP 1.631
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.801 SNIP 1.652 CiteScore 2.38
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.692 SNIP 1.751 CiteScore 1.95
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.822 SNIP 1.901 CiteScore 1.73
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.774 SNIP 1.666 CiteScore 1.42
ISI indexed (2012): ISI indexed yes
Electrochemistry of single molecules and biomolecules, molecular scale nanostructures, and low-dimensional systems

Electrochemistry at ultra-small scales, where even the single molecule or biomolecule can be characterized and manipulated, is on the way to a consolidated status. At the same time molecular electrochemistry is expanding into other areas of sophisticated nano- and molecular scale systems including molecular scale metal and semiconductor nanoparticles (NPs) and other nanostructures, e.g. nanotubes, “nanoflowers” etc.. The new structures offer both new electronic properties and highly confined novel charge transfer environments.

General information
State: Published
Organisations: Department of Chemistry, NanoChemistry, Organic Chemistry, Kazan National Research Technological University
Authors: Nazmutdinov, R. R. (Ekstern), Zinkicheva, T. T. (Ekstern), Zinkicheva, T. T. (Ekstern), Shermukhamedov, S. A. (Ekstern), Zhang, J. (Intern), Ulstrup, J. (Intern)
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Publication date: 2018
Main Research Area: Technical/natural sciences

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Journal: Current Opinion in Electrochemistry
Volume: 7
ISSN (Print): 2451-9103
Original language: English
Energy vs. density on paths toward exact density functionals

Recently, the progression toward more exact density functional theory has been questioned, implying a need for more formal ways to systematically measure progress, i.e. a “path”. Here I use the Hohenberg-Kohn theorems and the definition of normality by Burke et al. to define a path toward exactness and “straying” from the “path” by separating errors in ρ and E[ρ]. A consistent path toward exactness involves minimizing both errors. Second, a suitably diverse test set of trial densities ρ' can be used to estimate the significance of errors in ρ without knowing the exact densities which are often inaccessible. To illustrate this, the systems previously studied by Medvedev et al., the first ionization energies of atoms with Z = 1 to 10, the ionization energy of water, and the bond dissociation energies of five diatomic molecules were investigated using CCSD(T)/aug-cc-pV5Z as benchmark at chemical accuracy. Four functionals of distinct designs were used: B3LYP, PBE, M06, and S-VWN. For atomic cations regardless of charge and compactness up to Z = 10, the energy effects of the different ρ are < 4 kJ/mol (chemical accuracy) defined here as “normal”, even though these four functionals ranked very differently in the previous test. Thus, the “off-path” behavior for such cations is energy-wise insignificant. An interesting oscillating behavior in the density sensitivity is observed vs. Z, explained by orbital occupation effects. Finally, it is shown that even large “normal” problems such as the Co-C bond energy of cobalamins can use simpler (e.g. PBE) trial densities to drastically speed up computation by loss of a few kJ/mol in accuracy. The proposed method of using a test set of trial densities to estimate the sensitivity and significance of density errors of functionals may be useful for testing and designing new balanced functionals with more systematic improvement of densities and energies.
Flavins mediate extracellular electron transfer in Gram-positive Bacillus megaterium strain LLD-1

The extracellular electron transfer (EET) mechanism of an isolated Gram-positive Bacillus megaterium strain (LLD-1), identified by 16S rRNA gene sequencing and physiological analysis, was investigated in the present study. The electrochemical activity of strain LLD-1 was confirmed by electrochemical E-t and amperometric I-t tests. Flavins in culture suspension from strain LLD-1 were further proved to be able to act as electron shuttles, strengthening the electron transfer from LLD-1 to the electrode. The output voltage and current output were increased 2.8 times and 3.7 times, respectively, by adding 100 nM exogenetic flavins into microbial fuel cells inoculated with LLD-1. Electricity generation by LLD-1 from different carbon sources can be enhanced by adding 100 nM exogenetic flavins. This study indicated that flavins were essential to the EET process of the Gram-positive strain LLD-1. Furthermore, a putative EET model for B. megaterium strain LLD-1 and even for Gram-positive bacteria was proposed.
High-resolution synchrotron terahertz investigation of the large-amplitude hydrogen bond librational band of \( (\text{HCN})_2 \)

The high-resolution terahertz absorption spectrum of the large-amplitude intermolecular donor librational band \( \nu_8 \) of the homodimer \( (\text{HCN})_2 \) has been recorded by means of long-path static gas-phase Fourier transform spectroscopy at 207 K employing a highly brilliant electron storage ring source. The rovibrational structure of the \( \nu_8 \) band has the typical appearance of a perpendicular type band of a \( \Sigma-\Pi \) transition for a linear polyatomic molecule. The generated terahertz spectrum is analyzed employing a standard semi-rigid linear molecule Hamiltonian, yielding a band origin \( \nu_0 \) of
119.11526(60) cm$^{-1}$ together with values for the excited state rotational constant B', the excited state quartic centrifugal distortion constant D$_J''$ and the l-type doubling constant q for the degenerate state associated with the ν18 mode. The until now missing donor librational band origin enables the determination of an accurate experimental value for the vibrational zero-point energy of 2.50 ± 0.05 kJ mol$^{-1}$ arising from the entire class of large-amplitude intermolecular modes. The spectroscopic findings are complemented by CCSD(T)-F12b/aug-cc-pV5Z (electronic energies) and CCSD(T)-F12b/aug-cc-pVQZ (force fields) electronic structure calculations, providing a (semi)-experimental value of 17.20 ± 0.20 kJ mol$^{-1}$ for the dissociation energy D$_0$ of this strictly linear weak intermolecular CH⋯N hydrogen bond.

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Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
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Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.715 SNIP 1.216 CiteScore 4.05
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.916 SNIP 1.184 CiteScore 3.67
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BFI (2011): BFI-level 2
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ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.802 SNIP 1.196
Web of Science (2010): Indexed yes
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Scopus rating (2009): SJR 2.127 SNIP 1.369
Web of Science (2009): Indexed yes
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Scopus rating (2008): SJR 2.158 SNIP 1.211
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Scopus rating (2007): SJR 1.84 SNIP 1.138
Influence of Adsorption and Capillary Pressure on Phase Equilibria Inside Shale Reservoirs

Due to the small pore sizes and organic content of shale, capillary pressure and adsorption are two effects that should be taken into account in the study of phase equilibrium inside shale. The inclusion of both effects in the phase equilibrium modeling can shed light on how bulk phase composition inside the porous media changes with temperature and pressure, and how the phase equilibrium changes accordingly. In the long run, such a model can be used in reservoir simulation for more complicated analysis. In this study, we present a calculation method that can effectively include adsorption and capillarity. We propose to introduce an excess adsorbed phase and treat the remaining substance inside the pores as a bulk phase (gas, liquid, or both) in order to make the mass balance formulation simpler. The adsorbed phase is modeled by the Multicomponent Langmuir (ML) equation for its simplicity and computational efficiency. A more theoretical adsorption model, the multicomponent potential theory of adsorption (MPTA), is used to determine the parameters of the simpler ML equation. The liquid and gas phases are described by the Peng-Robinson equation of state and the capillary pressure across their interface is taken into account. A flash algorithm by alternately updating the adsorbed phase amount and the fugacities in the bulk phases has been developed. The flash algorithm is used to analyze some representative systems (from binary, ternary to low-GOR and high-GOR model reservoir fluid systems) for the phase equilibrium inside porous media. The results show that adsorption and capillary pressure can significantly change the bulk phase composition and thus its corresponding phase envelope. Since the adsorption varies at different temperature and pressure conditions, the extent of change in the phase envelope is different. In general, a much shrunk phase envelope with a shifted critical point is observed. The heavier components are preferentially adsorbed in the whole pressure and temperature range studied here. At high pressure and low temperature, the selectivity towards heavier components is moderate in comparison to the that at low pressure and high temperature. The adsorption effects are stronger for the gas bulk phase region, leading to bigger changes in the gas phase composition and the shift of the dew point curve. PVT simulations of two model reservoir fluid systems show significant change in the results when capillary pressure and adsorption are included.
Injectable iodine-125 labeled tissue marker for radioactive localization of non-palpable breast lesions

We have developed a 125I-radiolabeled injectable fiducial tissue marker with the potential to replace current methods used for surgical guidance of non-palpable breast tumors. Methods in routine clinical use today such as radioactive seed localization, radio-guided occult lesion localization and wire-guided localization suffers from limitations that this injectable fiducial tissue marker offers solutions to. The developed 125I-radiolabeled injectable fiducial tissue marker is based on highly viscous sucrose acetate isobutyrate. The marker was readily inserted in NMRI mice and proved to be spatially well-defined and stable over a seven day period with excellent CT contrast (>1500 HU), enabling fluoroscopic visualization of markers during placement. The radioactivity remains strongly associated with the marker during the implantation period, which limits exposure to healthy tissue. Biodistribution studies show that there is negligible radioactivity in all non-tumor tissues sampled, with the exception of the thyroid gland, where limited accumulation was observed (0.06% of injected dose after 7 days). Based on the excellent performance of the marker and the fact that it can be delivered through thin hypodermic needles (≥27G), the marker holds great promise for clinical application, since patient discomfort is reduced.
significantly compared to current methods. Statement of Significance. A new type of tissue marker for local administration to non-palpable breast tumors has been developed. The surgical guidance marker is based on derivatives of the biomaterial sucrose acetate isobutyrate and unlike currently used markers it is injectable in the tissue using thin needles, reducing the discomfort to the patients significantly. The marker confers CT contrast and has radioactive properties, meaning it also could find use in brachytherapy. The design of the iodine-125 labeled fiducial tissue marker enables control of dosimetry as well as a choice of iodine isotope used. The marker is anticipated to be clinical applicable due to its contrast performance in mice and its potential for enhanced flexibility in surgical procedures, compared to current methods.

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Web of Science (2015): Indexed yes
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Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.963 SNIP 2.269 CiteScore 6.41
ISI indexed (2013): ISI indexed yes
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BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.904 SNIP 2.125 CiteScore 5.51
ISI indexed (2012): ISI indexed yes
Scopus rating (2011): SJR 1.808 SNIP 1.91 CiteScore 5.15
ISI indexed (2011): ISI indexed yes
Scopus rating (2010): SJR 1.794 SNIP 1.964
Web of Science (2010): Indexed yes
Scopus rating (2009): SJR 1.399 SNIP 1.662
Scopus rating (2008): SJR 1.404 SNIP 1.981
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Interaction between structurally different heteroexopolysaccharides and β-lactoglobulin studied by solution scattering and analytical ultracentrifugation

Despite a very large number of bacterial exopolysaccharides have been reported, detailed knowledge on their molecular structures and associative interactions with proteins is lacking. Small-angle X-ray scattering, dynamic light scattering and analytical ultracentrifugation (AUC) were used to characterize the interactions of six lactic acid bacterial heteroexopolysaccharides (HePS-1-HePS-6) with β-lactoglobulin (BLG). Compared to free HePSs, a large increase in the X-ray radius of gyration RG, maximum length L and hydrodynamic diameter $d_H$ of HePS-1-HePS-4 mixed with BLG revealed strong aggregation, the extent of which depended on the compact conformation and degree of branching of these HePSs. No significant effects were observed with HePS-5 and HePS-6. Turbidity and AUC analyses showed that both soluble and insoluble BLG-HePS complexes were formed. The findings provide new insights into the role of molecular structures in associative interactions between HePSs and BLG which has relevance for various industrial applications.
Investigation of curing rates of bio-based thiol-ene films from diallyl 2,5-furandicaboxylate

The bio-based monomer, 2,5-furandicarboxylic acid, has been adapted to classic thiol-ene chemistry by derivatization of the acid with allyl alcohol. This new monomer has allowed for the synthesis of new thermoset systems, capable of forming green, sustainable materials through UV-crosslinking. In this study, the synthesis of the new monomer along with thorough kinetic studies of the new thermoset systems are presented. In order to determine kinetic values for the systems, all reactions have been followed by real-time FT-IR. Initially, a study of three different photoinitiators is performed on a classic TEMPIC-TATATO system, in order to determine the superior initiator for the new systems. The new monomer is crosslinked with five different thiol compounds in both stoichiometric and off-stoichiometric ratios, yielding an array of bio-based thermosets. The properties of these systems are determined through DSC, TGA and tensile testing, allowing determination of the systems with superior properties. In general, most systems proved to cure fully, with the exception of issues encountered from thiols with long ethoxylated chains.

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Authors: Larsen, D. B. (Intern), Sønderbæk-Jørgensen, R. (Ekstern), Duus, J. Ø. (Intern), Daugaard, A. E. (Intern)
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Web of Science (2015): Indexed yes
Iridium Catalysis: Reductive Conversion of Glucan to Xylan

By using iridium catalysed dehydrogenative decarbonylation, we converted a partly protected cellobioside into a fully protected xylobioside. We demonstrate good yields with two different aromatic ester protecting groups. The resulting xylobioside was directly used as glycosyl donor in further synthesis of a xylooctaose.

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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
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BFI (2011): BFI-level 2
Scopus rating (2011): SJR 2.857 SNIP 1.322 CiteScore 5.96
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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
Scopus rating (2006): SJR 2.366 SNIP 1.183
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 2.129 SNIP 1.15
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Scopus rating (2004): SJR 1.954 SNIP 1.158
Scopus rating (2003): SJR 1.644 SNIP 1.098
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 1.956 SNIP 1.19
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 1.817 SNIP 1.098
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Kinetic Analysis of Hexose Conversion to Methyl Lactate by Sn Beta: Effects of Substrate Masking and of Water

Simple sugars bear promise as substrates for the formation of fuels and chemicals using heterogeneous catalysts in alcoholic solvents. Sn-Beta is a particularly well suited catalyst for the cleavage, isomerization and dehydration of sugars into more valuable chemicals. In order to understand these processes and save resources and time by optimising them, kinetic and mechanistic analyses are helpful. Herein, we study substrate entry into the Sn-Beta catalysed methyl lactate process using abundant hexose substrates. NMR spectroscopy is applied to show that the formation of methyl lactate occurs in two kinetic regimes for fructose, glucose and sucrose. The majority of methyl lactate is not formed from the substrate directly, but from methyl fructosides in a slow regime. At 160 °C, more than 40% of substrate carbon are masked (i.e. reversibly protected in situ) as methyl fructosides within few minutes when using hydrothermally synthesised Sn-Beta, while more than 60% methyl fructosides can be produced within few minutes using post synthetically synthesised Sn-Beta. A significant fraction of substrate thus is masked by rapid methyl fructoside formation prior to subsequent slow release of fructose. This release is the rate limiting step in the Sn-Beta catalysed methyl lactate process, but can be accelerated by the addition of small amounts of water at the expense of maximum methyl lactate yield.

Metabolic fate of ¹³C-labelled polydextrose and impact on the gut microbiome: A triple-phase study in a colon simulator

The present study introduces a novel triple-phase (liquids, solids and gases) approach, which employed uniformly labelled [U-¹³C] polydextrose (PDX) for the selective profiling of metabolites generated from dietary fiber fermentation in an in vitro colon simulator using human fecal inocula. Employing [¹³C] NMR spectroscopy, [U-¹³C] PDX metabolism was observed from colonic digest samples. The major ¹³C-labelled metabolites generated were acetate, butyrate, propionate, and valerate. In addition to these short-chain fatty acids (SCFAs), ¹³C-labelled lactate, formate, succinate,
and ethanol were detected in the colon simulator samples. Metabolite formation and PDX substrate degradation were examined comprehensively over time (24 and 48 hours). Correlation analysis between $^{13}$C NMR spectra and gas production confirmed the anaerobic fermentation of PDX to SCFAs. In addition, 16S rRNA gene analysis showed that the level of Erysipelotrichaceae was influenced by PDX supplementation and Erysipelotrichaceae level were statistically correlated with SCFA’s formation. Overall, our study demonstrates a novel approach to link substrate fermentation and microbial function directly in a simulated colonic environment.

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Authors: Lamichhane, S. (Ekstern), Yde, C. C. (Ekstern), Max Jensen, H. (Ekstern), Morovic, W. (Ekstern), Hibberd, A. A. (Ekstern), Ouwehand, A. C. (Ekstern), Saarinen, M. T. (Ekstern), Forssten, S. D. (Ekstern), Wiebe, L. (Ekstern), Marcussen, J. (Ekstern), Bertelsen, K. (Ekstern), Meier, S. (Intern), Young, J. F. (Ekstern), Bertram, H. C. (Ekstern)  
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Scopus rating (2013): SJR 2.002 SNIP 1.256 CiteScore 5.16  
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Scopus rating (2012): SJR 2.027 SNIP 1.328 CiteScore 5.12  
ISI indexed (2012): ISI indexed yes  
Web of Science (2012): Indexed yes  
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Scopus rating (2011): SJR 2.119 SNIP 1.267 CiteScore 5.12  
ISI indexed (2011): ISI indexed yes  
BFI (2010): BFI-level 2  
Scopus rating (2010): SJR 1.93 SNIP 1.246  
Web of Science (2010): Indexed yes  
BFI (2009): BFI-level 2  
Scopus rating (2009): SJR 1.959 SNIP 1.206  
BFI (2008): BFI-level 2  
Scopus rating (2008): SJR 1.993 SNIP 1.122  
Web of Science (2008): Indexed yes  
Scopus rating (2007): SJR 1.921 SNIP 1.108  
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Methanation of CO₂ over Zeolite-Encapsulated Nickel Nanoparticles

Efficient methanation of CO₂ relies on the development of more selective and stable heterogeneous catalysts. Here we present a simple and effective method to encapsulate Ni nanoparticles in zeolite silicalite-1. In this method, the zeolite is modified by selective desilication, which creates intra-particle voids and mesopores that facilitate the formation of small and well-dispersed nanoparticles upon impregnation and reduction. TEM and XPS analysis confirm that a significant part of the Ni nanoparticles are situated inside the zeolite rather than on the outer surface. The encapsulation results in an increased metal dispersion and, consequently, a high catalytic activity for CO₂ methanation. With a gas hourly space velocity of 60000 ml/g catalyst h⁻¹ and H₂/CO₂=4, the zeolite-encapsulated Ni nanoparticles result in 60% conversion at 450°C, which corresponds to a site-time yield of around 304 mol CH₄/mol Ni h⁻¹. The encapsulated Ni nanoparticles show no change in activity or selectivity after 50 h of operation, although post-catalysis characterisation reveals some particle migration.

General information

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Authors: Goodarzi, F. (Intern), Kang, L. (Ekstern), Wang, F. R. (Ekstern), Joensen, F. (Ekstern), Kegnæs, S. (Intern), Mielby, J. J. (Intern)
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Web of Science (2014): Indexed yes
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Web of Science (2013): Indexed yes
Scopus rating (2016): CiteScore 4.33 SJR 1.636 SNIP 0.932
Web of Science (2016): Indexed yes
Scopus rating (2015): SJR 1.751 SNIP 1 CiteScore 4.57
Web of Science (2015): Indexed yes
Scopus rating (2014): SJR 1.88 SNIP 1.102 CiteScore 4.52
Web of Science (2014): Indexed yes
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
Modeling magnetic circular dichroism within the polarizable embedding approach

Magnetic circular dichroism (MCD) is defined as the differential absorption of left and right circularly polarized light in a sample subjected to an external magnetic field. In order to interpret the results of MCD measurements, theoretical predictions of key MCD parameters can be of utmost importance. From an experimental point of view, MCD spectra of molecules are often measured in an environment and most notably in a solution. Thus, it may be very important that the method used to predict the MCD parameters is able to correctly account for medium effects. In this paper, we investigate the quality of MCD calculations within the polarizable embedding approach, which represents a fully atomistic and polarizable representation of an environment surrounding a smaller region treated using quantum mechanics. Furthermore, we compare the performance of the polarizable embedding scheme to the use of the more conventional dielectric continuum approach. Results are presented for cytosine and hypoxanthine solvated in water.

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Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.668 SNIP 0.611 CiteScore 1.49
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Scopus rating (2013): SJR 0.763 SNIP 0.663 CiteScore 1.76
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.989 SNIP 0.807 CiteScore 2.05
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.47 SNIP 1.227 CiteScore 3.16
ISI indexed (2011): ISI indexed yes
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BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.293 SNIP 0.923
Web of Science (2010): Indexed yes
Near-wellbore modeling of a horizontal well with Computational Fluid Dynamics

The oil production by horizontal wells is a complex phenomenon that involves flow through the porous reservoir, completion interface and the well itself. Conventional reservoir simulators can hardly resolve the flow through the completion into the wellbore. On the contrary, Computational Fluid Dynamics (CFD) is capable of modeling the complex interaction between the creeping reservoir flow and turbulent well flow for single phases, while capturing both the completion geometry and formation damage. A series of single phase steady-state simulations are undertaken, using such fully coupled three dimensional numerical models, to predict the inflow to the well. The present study considers the applicability of CFD for near-wellbore modeling through benchmark cases with available analytical solutions. Moreover, single phase steady-state numerical investigations are performed on a specific perforated horizontal well producing from the Siri field, offshore Denmark. The performance of the well is investigated with an emphasis on the inflow profile and the productivity index for different formation damage scenarios. A considerable redistribution of the inflow profile were found when the filtrate invasion extended beyond the tip of the perforations.

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State: Published
Organisations: Department of Mechanical Engineering, Scientific Computing, Fluid Mechanics, Coastal and Maritime Engineering, Department of Chemistry, CERE – Center for Energy Resources Engineering, Technical University of Denmark, Lloyd’s Register Consulting
Authors: Szanyi, M. L. (Ekstern), Hemmingsen, C. S. (Intern), Yan, W. (Intern), Walther, J. H. (Intern), Glimberg, S. L. (Ekstern)
Pages: 119-128
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Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Petroleum Science and Engineering
Volume: 160
ISSN (Print): 0920-4105
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.56 SJR 0.764 SNIP 1.631
On the biosynthetic origin of carminic acid

The chemical composition of the scale insect Dactylopius coccus was analyzed with the aim to discover new possible intermediates in the biosynthesis of carminic acid. UPLC-DAD/HRMS analyses of fresh and dried insects resulted in the identification of three novel carminic acid analogues and the verification of several previously described intermediates. Structural elucidation revealed that the three novel compounds were desoxyerythrolaccin-O-glucosyl (DE-O-Glcp), 5,6-didehydroxyerythrolaccin 3-O-β-D-glucopyranoside (DDE-3-O-Glcp), and flavokermesic acid anthrone (FKA). The finding of FKA in D. coccus provides solid evidence of a polyketide, rather than a shikimate, origin of coccid pigments. Based on the newly identified compounds, we present a detailed biosynthetic scheme that accounts for the formation of carminic acid (CA) in D. coccus and all described coccid pigments which share a flavokermesic acid anthrone (FKA) core. Detection of coccid pigment intermediates in members of the Planococcus (mealybugs) and Pseudaulacaspis genera shows that the ability to...
form these pigments is taxonomically more widely spread than previously documented. The shared core-FK-biosynthetic pathway and wider taxonomic distribution suggests a common evolutionary origin for the trait in all coccid dye producing insect species.

**General information**

State: Accepted/In press
Organisations: Department of Biotechnology and Biomedicine, Department of Chemistry, Organic Chemistry, Eukaryotic Molecular Cell Biology, Natural Product Discovery, Biosynthetic Pathway Engineering, University of Copenhagen, Chr. Hansen AS
Number of pages: 28
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Main Research Area: Technical/natural sciences

**Publication information**

Journal: Insect Biochemistry and Molecular Biology
ISSN (Print): 0965-1748
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.69 SJR 1.845 SNIP 1.049
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.917 SNIP 1.135 CiteScore 3.75
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.62 SNIP 1.214 CiteScore 3.59
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.688 SNIP 1.348 CiteScore 3.87
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.616 SNIP 1.192 CiteScore 3.56
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.682 SNIP 1.311 CiteScore 3.54
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.736 SNIP 1.309
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.575 SNIP 1.009
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.286 SNIP 1.004
Scopus rating (2007): SJR 1.582 SNIP 1.131
Scopus rating (2006): SJR 1.419 SNIP 1.012
Scopus rating (2005): SJR 1.421 SNIP 1.063
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.363 SNIP 1.004
Scopus rating (2003): SJR 1.443 SNIP 1.118
Scopus rating (2002): SJR 1.182 SNIP 1.126
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.935 SNIP 1.013
Potassium and soot interaction in fast biomass pyrolysis at high temperatures

This study aims to investigate the interaction between potassium and carbonaceous matrix of soot produced from wood and herbaceous biomass pyrolysis at high heating rates at 1250°C in a drop tube reactor. The influence of soot carbon chemistry and potassium content in the original biomass on the CO2 reactivity was studied by thermogravimetric analysis. The XPS results showed that potassium incorporation with oxygen-containing surface groups in the soot matrix did not occur during high temperature pyrolysis. The potassium was mostly found as water-soluble salts such as KCl, KOH, KHC\textsubscript{3}O\textsubscript{3}, and K\textsubscript{2}CO\textsubscript{3} in herbaceous biomass soot. The low ash-containing pinewood soot was less reactive than the potassium rich herbaceous biomass soot, indicating a dominating role of potassium on the soot reactivity. However, the catalytic effect of potassium on the reactivity remained the same after a certain potassium amount was incorporated in the soot matrix during pyrolysis. Raman spectroscopy results showed that the carbon chemistry of biomass soot also affected the CO\textsubscript{2} reactivity. The less reactive pinewood soot was more graphitic than herbaceous biomass soot samples with the disordered carbon structure.
Prodrugs activated by reactive oxygen species for use in the treatment of inflammatory diseases and cancer

Prodrugs activated predominantly or exclusively in inflammatory tissue, more particularly prodrugs of methotrexate and derivatives thereof, which are selectively activated by Reactive Oxygen Species (ROS) in inflammatory tissues associated with cancer and inflammatory diseases, as well as method for preparing said prodrugs.

General information

State: Published
Organisations: Department of Chemistry, Organic Chemistry
Authors: Peiro Cadahia, J. (Ekstern), Clausen, M. H. (Intern), Bondebjerg, J. (Ekstern), Hansen, C. A. (Ekstern), Andersen, N. S. (Ekstern)
Publication date: 2018

Publication information
IPC: A61K31/519; A61P29/00; A61P35/00; C07D487/04
Patent number: WO2018037119
Date: 01/03/2018
Priority date: 26/08/2016
Priority number: EP20160185889
Original language: English
Electronic versions:
WO2018037119A1.pdf
Main Research Area: Technical/natural sciences
Publication: Research - Patent – Annual report year: 2018
RAND-Based Formulations for Isothermal Multiphase Flash

Two algorithms are proposed for isothermal multiphase flash. These are referred to as modified RAND and vol-RAND. The former uses the chemical potentials and molar-phase amounts as the iteration variables, while the latter uses chemical potentials and phase volumes to cosolve a pressure-explicit equation of state (EOS) with the equilibrium equations. Compared with the conventional second-order approach using Gibbs-energy minimization, these methods are more structured, with all components in all phases treated in the same way. Both have been derived to include chemical reactions for any number of phases along with the possible simplifications for only phase equilibria. The simple structured implementation of these methods is demonstrated for modified RAND and vol-RAND. The rate of convergence of the methods presented is shown to be the same as the conventional second-order method for isothermal flash. It is demonstrated that the use of an association term [cubic plus association (CPA)] adds little additional computational cost when using vol-RAND compared with a simple cubic Soave-Redlich-Kwong (SRK) without association. The RAND methods scale better in terms of the $O(n^2)$ operations as more phases are introduced, and are computationally less expensive than the conventional Gibbs minimization method for more than three phases.

General information
State: Accepted/In press
Organisations: Department of Chemistry, Department of Chemical and Biochemical Engineering
Authors: Paterson, D. (Intern), Michelsen, M. L. (Intern), Stenby, E. H. (Intern), Yan, W. (Intern)
Number of pages: 15
Publication date: 2018
Conference: SPE Reservoir Simulation Conference, Montgomery Texas, United States, 20/02/2017 - 20/02/2017
Main Research Area: Technical/natural sciences

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Journal: Spe Journal
Article number: SPE-182706-PA
ISSN (Print): 1086-055X
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.01 SJR 0.95 SNIP 2.003
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.976 SNIP 1.838 CiteScore 2.37
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.185 SNIP 2.152 CiteScore 2.43
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.993 SNIP 1.773 CiteScore 2.25
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.047 SNIP 1.757 CiteScore 2.13
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.139 SNIP 1.757 CiteScore 2.3
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.143 SNIP 2.103
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.106 SNIP 1.642
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.513 SNIP 1.369
Remote-loading of liposomes with manganese-52 and in vivo evaluation of the stabilities of $^{52}$Mn-DOTA and $^{64}$Cu-DOTA using radiolabelled liposomes and PET imaging

Liposomes are nanoparticles used in drug delivery that distribute over several days in humans and larger animals. Radiolabeling with long-lived positron emission tomography (PET) radionuclides, such as manganese-52 ($^{52}$Mn, T½=5.6 days), allow the imaging of this biodistribution. We report optimized protocols for radiolabeling liposomes with $^{52}$Mn, through both remote-loading and surface labeling. For comparison, liposomes were also remote-loaded and surface labeled with copper-64 ($^{64}$Cu, T½=12.7h) through conventional means. The chelator DOTA was used in all cases. The in vivo stability of radionmetal chelates is widely debated but studies that mimic a realistic in vivo setting are lacking. Therefore, we employed these four radiolabeled liposome types as platforms to demonstrate a new concept for such in vivo evaluation, here of the chelates $^{52}$Mn-DOTA and $^{64}$Cu-DOTA. This was done by comparing "shielded" remote-loaded with "exposed" surface labeled variants in a CT26 tumor-bearing mouse model. Remote loading (90min at 55°C) and surface labeling (55°C for 2h) of $^{52}$Mn gave excellent radiolabeling efficiencies of 97-100% and 98-100% respectively, and the liposome biodistribution was imaged by PET for up to 8days. Liposomes with surface-conjugated $^{52}$Mn-DOTA exhibited a significantly shorter plasma half-life (T½=14.4h) when compared to the remote-loaded counterpart (T½=21.3h), whereas surface-conjugated $^{64}$Cu-DOTA cleared only slightly faster and non-significantly, when compared to remote-loaded (17.2±2.9h versus 20.3±1.2h). From our data, we conclude the successful remote-loading of liposomes with $^{52}$Mn, and furthermore that $^{52}$Mn-DOTA may be unstable in vivo whereas $^{64}$Cu-DOTA appears suitable for quantitative imaging.

General information
State: Published
Organisations: Center for Nuclear Technologies, The Hevesy Laboratory, Department of Micro- and Nanotechnology, Colloids and Biological Interfaces, Department of Chemistry, University of Copenhagen
Pages: 100-109
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Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Controlled Release
Volume: 269
ISSN (Print): 0168-3659
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 7.56 SJR 2.393 SNIP 1.84
Selective Hydrodeoxygenation of Alkyl Lactates to Alkyl Propionates with Fe-based Bimetallic Supported Catalysts

Hydrodeoxygenation (HDO) of methyl lactate (ML) to methyl propionate (MP) was performed with various base-metal supported catalysts. A high yield of 77% MP was obtained with bimetallic Fe-Ni/ZrO₂ in methanol at 220°C and 50 bar H₂. A synergistic effect of Ni increased the yield of MP significantly when using Fe-Ni/ZrO₂ instead of Fe/ZrO₂ alone. Moreover, the ZrO₂ support contributed to improve the yield as a phase transition of ZrO₂ from tetragonal to monoclinic occurred after metal doping giving rise to fine dispersion of the Fe and Ni on the ZrO₂, resulting in a higher catalytic activity of the material. Interestingly, it was observed that Fe-Ni/ZrO₂ also effectively catalyzed methanol reforming to produce H₂ in situ, followed by HDO of ML, yielding 60% MP at 220°C with 50 bar N₂ instead of H₂. Fe-Ni/ZrO₂ also catalyzed HDO of other short-chain alkyl lactates to the corresponding alkyl propionates in high yields around 70%. No loss of activity of Fe-Ni/ZrO₂ occurred in five consecutive reaction runs demonstrating the high durability of the catalyst system.
Selective Oxidative Carbonylation of Aniline to Diphenylurea with Ionic Liquids
A catalytic system for the selective oxidative carbonylation of aniline to diphenylurea based on Pd complexes in combination with imidazolium ionic liquids is presented. Both oxidants, Pd complexes and ionic liquids affect the activity of the reaction while the choice of oxidant determines the selectivity of the reaction. Together they allow the reaction to proceed under comparatively mild conditions without loss of activity. In-situ NMR examination of the reaction led to the observation of a previously suggested intermediate supporting the proposed mechanism.

General information
State: Accepted/In press
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry, Universitat Rovira i Virgili
Authors: Zahrtmann, N. (Intern), Claver, C. (Ekstern), Godard, C. (Ekstern), Riisager, A. (Intern), Garcia Suárez, E. J. (Intern)
Number of pages: 11
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information
Journal: ChemCatChem
ISSN (Print): 1867-3880
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Web of Science (2016): Indexed yes
Scopus rating (2016): CiteScore 4.33 SJR 1.636 SNIP 0.932
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
Web of Science (2010): Indexed yes
Original language: English
DOIs:
10.1002/cctc.201800004
Publication: Research - peer-review › Journal article – Annual report year: 2018

Silylative Pinacol Coupling Catalyzed by Nitrogen-Doped Carbon-Encapsulated Nickel/Cobalt Nanoparticles: Evidence for a Silyl Radical Pathway
The silylative pinacol coupling of arylaldehydes catalyzed by an easily accessible, heterogeneous base-metal catalyst is demonstrated. Instead of using the classical combination of catalyst, stoichiometric metal reductants, and chlorosilanes, the developed reaction only requires the use of a catalyst and a hydrosilane, which serves as both reductant and silylating agent. A rare mechanistic investigation in this field focusing on the organic reactants was undertaken using various techniques including experimental rate orders, kinetic isotope effect, radical scavengers, and stoichiometric tests. The obtained results provided evidence for a reaction mechanism which is different from the classical pinacol coupling pathway. We propose that the heterogeneous catalyst facilitates easy access to silyl radicals, thereby circumventing the
usual need for explosive initiators to access these species. In addition, leaching tests and recycling of the catalyst were performed, clearly supporting the heterogeneous nature of the catalyst.

**General information**
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry
Authors: Kramer, S. (Intern), Hejjo, F. (Intern), Rasmussen, K. H. (Intern), Kegnæs, S. (Intern)
Pages: 754-759
Publication date: 2018
Main Research Area: Technical/natural sciences

**Publication information**
Journal: ACS Catalysis
Volume: 8
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**Ratings:**
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 10.3 SJR 4.299 SNIP 2.071
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 4.039 SNIP 2.134 CiteScore 9.88
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 3.641 SNIP 2.022 CiteScore 8.74
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 3.271 SNIP 1.859 CiteScore 7.41
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Scopus rating (2012): SJR 2.684 SNIP 1.61 CiteScore 5.19
ISI indexed (2012): ISI indexed no
Web of Science (2012): Indexed yes
ISI indexed (2011): ISI indexed no
Original language: English
Heterogeneous catalysis, Nanoparticles, Nitrogen-doped carbon, Mechanism, Silyl radicals

**DOIs:**
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Source: FindIt
Source-ID: 2394007928
Publication: Research - peer-review → Journal article – Annual report year: 2018

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**Site-Specific Reactivity of Copper Chabazite Zeolites with Nitric Oxide, Ammonia, and Oxygen**

In-situ electron paramagnetic resonance (EPR) spectroscopy was applied to dilute copper chabazite (CHA) zeolites under gas flows relevant for the selective catalytic reduction of NO with ammonia (NH3-SCR). Under both reducing and oxidizing conditions, we observed differences in reactivity between the different monomeric copper sites present: When reducing with NO+NH3, the rate of reduction of Cu2+ sites depends on NH3 coverage. The subsequent oxidation with O2 results in a clean EPR spectrum of only one type of copper site, whereas oxidation in NO+O2 gives two types of copper sites. The rate of oxidation differs significantly between reaction with O2 alone and with NO+O2 together. Thus it was revealed that [Cu(NH3)2]+ complexes, which are regarded to be only weakly associated with the framework, nevertheless have different reactivity depending on the Al distribution in the proximity. The observed differences in reactivity of copper sites has implications for the mechanistic understanding of NH3-SCR with Cu-zeolites.

**General information**
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Technical University of Denmark, Haldor Topsoe AS
The aim of this paper was to perform a comprehensive characterization of polysaccharides isolated from the interior (IOI) and exterior (IOE) parts of the fungus *Inonotus obliquus*. Pre-extraction with DCM and MeOH, followed by water and alkali extraction and ethanol precipitation gave two water extracts and two alkali extracts. Neutral and acidic polysaccharide fractions were obtained after anion-exchange chromatography of the water extracts. The neutral polysaccharides (60–73kDa) were heterogeneous and branched and consisted of a (1→3)-linked β-Glc backbone with (1→6)-linked kinks in the chain at approximately every fifth residue, with branches of (1→6)-linked β-Glc in addition to substantial amounts of (1→6)-linked α-Gal with 3-O-methylation at about every third Gal residue. The acidic polysaccharide fractions (10–31kDa) showed similar structural motifs as the neutral fractions differing mainly by the presence of (1→4)-linked α-GalA and α-GlcA, β-Xyl, α-Man and α-Rha were also present in varying amounts in all fractions. No major structural differences between the IOI and IOE fractions were observed. An alkaline polysaccharide fraction (>450kDa) was obtained from the IOI alkali extract, and consisted mainly of (1→3)- and (1→6)-linked β-Glc and (1→4)-linked β-Xyl. Several of the fractions showed in vitro immunomodulatory effect by increasing NO production in the murine macrophage and dendritic cell lines J774.A1 and D2SC/1. Most fractions managed to increase NO production only at the highest concentration tested (100μg/ml), while the neutral fraction IOE-WN activated potent NO production at 10μg/ml and was considered the most promising immunomodulating fraction in this study.
Synthesis of branched and linear 1,4-linked galactan oligosaccharides

We report the synthesis of linear and branched (1→4)-D-galactans. Four tetra- and one pentasaccharide were accessed by adopting a procedure of regioselective ring opening of a 4,6-O-naphthylidene protecting group followed by glycosylation using phenyl thioglycoside donors. The binding of the linear pentasaccharide with galectin-3 is also investigated by determination of a co-crystal structure. The binding of the (1→4)-linked galactan to Gal-3 highlights oligosaccharides of pectic galactan, which is abundant in the human diet, as putative Gal-3 ligands.

General information

State: Accepted/In press
Organisations: Department of Chemistry, Organic Chemistry, University of Copenhagen, SARomics Biostructure AB, Newcastle University
Number of pages: 14
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information

Journal: Organic and Biomolecular Chemistry
ISSN (Print): 1477-0520
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.39 SJR 1.363 SNIP 0.803
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.41 SNIP 0.858 CiteScore 3.47
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.387 SNIP 0.903 CiteScore 3.5
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.481 SNIP 0.897 CiteScore 3.55
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.635 SNIP 0.934 CiteScore 3.47
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.737 SNIP 0.974 CiteScore 3.71
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
Synthesis of Two Tetrasaccharide Pentenyl Glycosides Related to the Pectic Rhamnogalacturonan I Polysaccharide

The synthesis of two protected tetrasaccharide pentenyl glycosides with diarabinan and digalactan branching related to the pectic polysaccharide rhamnogalacturonan I is reported. The strategy relies on the coupling of N-phenyl trifluoroacetimidate disaccharide donors to a common rhamnosyl acceptor. The resulting trisaccharide thioglycosides were finally coupled to an n-pentenyl galactoside acceptor to access the two protected branched tetrasaccharides.

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry, Technical University of Denmark
Authors: Zakharova, A. N. (Ekstern), Awan, S. I. (Intern), Nami, F. (Intern), Gotfredsen, C. H. (Intern), Madsen, R. (Intern), Clausen, M. H. (Intern)
Number of pages: 14
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information
Journal: Molecules
Volume: 23
Issue number: 2
Article number: 327
ISSN (Print): 1420-3049
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.09 SJR 0.809 SNIP 1.231
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.562 SNIP 1.168 CiteScore 2.65
Tailored Electron Transfer Pathways in Aucore/Ptshell -Graphene Nanocatalysts for Fuel Cells

Au(core)Pt(shell)-graphene catalysts (G-Cys-Au@Pt) are prepared through chemical and surface chemical reactions. Au–Pt core–shell nanoparticles (Au@Pt NPs) covalently immobilized on graphene (G) are efficient electrocatalysts in low-temperature polymer electrolyte membrane fuel cells. The 9.5 ± 2 nm Au@Pt NPs with atomically thin Pt shells are attached on graphene via L-cysteine (Cys), which serves as linkers controlling NP loading and dispersion, enhancing the Au@Pt NP stability, and facilitating interfacial electron transfer. The increased activity of G-Cys-Au@Pt, compared to non-chemically immobilized G-Au@Pt and commercial platinum NPs catalyst (C–Pt), is a result of (1) the tailored electron transfer pathways of covalent bonds integrating Au@Pt NPs into the graphene framework, and (2) synergetic electronic effects of atomically thin Pt shells on Au cores. Enhanced electrocatalytic oxidation of formic acid, methanol, and ethanol is observed as higher specific currents and increased stability of G-Cys-Au@Pt compared to G-Au@Pt and C–Pt. Oxygen reduction on G-Cys-Au@Pt occurs at 25 mV lower potential and 43 A gPt−1 higher current (at 0.9 V vs reversible hydrogen electrode) than for C–Pt. Functional tests in direct fomic acid, methanol and ethanol fuel cells exhibit 95%, 53%, and 107% increased power densities for G-Cys-Au@Pt over C–Pt, respectively.

General information

State: Accepted/In press
Organisations: Department of Chemistry, NanoChemistry, Organic Chemistry, Tianjin University, Danish Power Systems Ltd.
The Molecular Mechanism of Alternative P450-Catalyzed Metabolism of Environmental Phenolic Endocrine-Disrupting Chemicals

Understanding the bioactivation mechanisms to predict toxic metabolites is critical for risk assessment of phenolic endocrine-disrupting chemicals (EDCs). One mechanism involves ipso-substitution, which may contribute to the total turnover of phenolic EDCs, yet the detailed mechanism and its relationship with other mechanisms are unknown. We used density functional theory to investigate the P450-catalyzed ipso-substitution mechanism of the prominent xenoestrogen bisphenol A. The ipso-substitution proceeds via H-abstraction from bisphenol A by Compound I, followed by essentially barrierless OH-rebound onto the ipso-position forming a quinol, which can spontaneously decompose into the carbocation and hydroquinone. This carboxylation can further evolve into the highly estrogenic hydroxylated and dimer-type metabolites. The H-abstraction/OH-rebound reaction mechanism has been verified as a general reaction mode for many other phenolic EDCs, such as bisphenol analogues, alkylphenols and chlorophenols. The identified mechanism enables us to effectively distinguish between type I (eliminating-substituent as anion) and type II (eliminating-substituent as cation) ipso-substitution in various phenolic EDCs. We envision that the identified pathways will be applicable for prediction of metabolites from phenolic EDCs whose fate is affected by this alternative type of P450 reactivity, and accordingly enable the screening of these metabolites for endocrine-disrupting activity.
Three-Dimensional Graphene Matrix-Supported and Thylakoid Membrane-Based High-Performance Bioelectrochemical Solar Cell

A combination of thylakoid membranes (TMs) as photobiocatalysts with high-surface-area electroactive materials could hold great potential for sustainable "green" solar energy conversion. We have studied the orientated immobilization of TMs on high-surface-area graphene electrodes, which were fabricated by electroreduction of graphene oxide and simultaneous electrodeposition with further aminooraryl functionalization. We have achieved the highest performance to date under direct electron transfer conditions through a biocompatible "wiring" of TMs to graphene sheets. The photo-biocurrent density generated by the optimized mediator-free TM-based bioanodes yielded up to 5.24 ± 0.50 μA cm⁻².

The photobioelectrochemical cell integrating the photobioanode in combination with an oxygen reducing enzymatic biocathode delivered a maximum power output of 1.79 ± 0.19 μW cm⁻². Our approach ensures a simplified cell design, a greater load of photosynthetic units, a minimized overpotential loss, and an enhanced overall performance.

Vanadium-Catalyzed Deoxydehydration of Glycerol Without an External Reductant

A vanadium‐catalysed deoxydehydration (DODH) of neat glycerol has been developed. Cheap and readily available ammonium metavanadate (NH₄VO₃) affords higher yields of allyl alcohol than the well‐established catalyst methyltrioxorhenium. A study in which deuterium-labelled glycerol was used was undertaken to further elucidate the dual role of glycerol as both an oxidant and reductant. This study led to the proposal of a metal-catalysed DODH mechanism for the production of allyl alcohol and a deeper understanding of the formation of the byproducts acrolein and propanal.
Vapor pressure and specific electrical conductivity in the solid and molten H₂O-CsH₂PO₄-CsPO₃ system—a novel electrolyte for water electrolysis at ~ 225–400 °C

Cesium dihydrogen phosphate, CsH₂PO₄ (CDP) was studied for water electrolysis at ~ 225–400 °C. In the presence of sufficient humidity, CDP is structurally disordered and super-protonic conducting with conductivities reaching 0.2–0.25 S cm⁻¹, when determined in suitable H-shaped sealed conductivity cells. Freshly prepared 99.7 ± 0.3% gravimetric pure CDP with correct X-ray diffraction and DSC diagram melted at ~ 345 °C. The vapor pressures, above CDP alone and mixed with 20–50 mol% CsPO₃ or 13 mol% H₂O, were determined in sealedampoules up to 355 °C by means of Raman spectroscopy based on internal reference gases. Pressures up to ~ 49 bar were estimated, much higher than previously expected. Conductivities were given as polynomials and plotted in solid and liquid states. Water splitting electrolysis 2H₂O → 2H₂ + O₂ was demonstrated by Raman at ~ 355 °C under a water pressure of ~ 23 bar in a quartz cell with platinum electrodes, showing molten CDP to have significant potential for water electrolysis.

General information
State: Accepted/In press
Organisations: Department of Energy Conversion and Storage, Proton conductors, Department of Chemistry
Authors: Nikiforov, A. V. (Intern), Berg, R. W. (Intern), Bjerrum, N. J. (Intern)
Number of pages: 22
Publication date: 2018
Main Research Area: Technical/natural sciences

Publication information
Journal: Ionics
ISSN (Print): 0947-7047
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
CRYSTAL STRUCTURE OF HUMAN DOPAMINE BETA-HYDROXYLASE

A crystalline form of dopamine β-hydroxylase is provided. X-ray crystallography reveals the space group and cell dimensions, as well as the atomic coordinates. The information can be used for identifying one or more modulators of dopamine β-hydroxylase, which can then be chemically synthesised and used in treatment. A process for preparing the crystalline form of human dopamine β-hydroxylase is also provided.

General information
State: Published
Organisations: Department of Chemistry, Metalloprotein Chemistry and Engineering, Københavns Universitet
Authors: Harris, P. H. (Forskerdatabase), Christensen, H. E. M. (Intern), Vendelboe, T. V. (Intern)
Dynamics of bad-cavity-enhanced interaction with cold Sr atoms for laser stabilization
Hybrid systems of cold atoms and optical cavities are promising systems for increasing the stability of laser oscillators used in quantum metrology and atomic clocks. In this paper we map out the atom-cavity dynamics in such a system and demonstrate limitations as well as robustness of the approach. We investigate the phase response of an ensemble of cold Sr88 atoms inside an optical cavity for use as an error signal in laser frequency stabilization. With this system we realize a regime where the high atomic phase shift limits the dynamical locking range. The limitation is caused by the cavity transfer function relating input field to output field. The cavity dynamics is shown to have only little influence on the prospects for laser stabilization, making the system robust towards cavity fluctuations and ideal for the improvement of future narrow linewidth lasers.

General information
State: Published
Organisations: Department of Chemistry, University of Copenhagen
Authors: Schäffer, S. A. (Intern), Christensen, B. T. (Ekstern), Henriksen, M. R. (Ekstern), Thomsen, J. W. (Ekstern)
Number of pages: 10
Publication date: 24 Jul 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Physical Review A
Volume: 96
Issue number: 1
Article number: 013847
ISSN (Print): 2469-9926
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
Scopus rating (2016): CiteScore 2.25 SJR 1.281 SNIP 0.852
Web of Science (2016): Indexed yes
Scopus rating (2015): SJR 1.451 SNIP 0.903 CiteScore 2.06
Web of Science (2015): Indexed yes
Scopus rating (2014): SJR 2.121 SNIP 1.146 CiteScore 2.46
Web of Science (2014): Indexed yes
Scopus rating (2013): SJR 2.317 SNIP 1.179 CiteScore 2.86
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Scopus rating (2012): SJR 2.515 SNIP 1.239 CiteScore 2.81
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
Scopus rating (2011): SJR 2.31 SNIP 1.261 CiteScore 2.79
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
Scopus rating (2010): SJR 2.403 SNIP 1.22
Friedel's salt profiles from thermogravimetric analysis and thermodynamic modelling of Portland cement-based mortars exposed to sodium chloride solution

Thermogravimetric analysis (TGA), powder X-ray diffraction (XRD) and thermodynamic modelling have been used to obtain Friedel's salt profiles for saturated mortar cylinders exposed to a 2.8 M NaCl solution. Comparison of the measured Friedel's salt profiles with the total chloride profiles indicates that only a minor part of the chloride ions is bound in Friedel's salt in the studied Portland cement (P) and limestone blended (L) cement. The chloride binding capacity with respect to the formation of Friedel's salt by consumption of monocarbonate is reached for the P and L mortars, where only a fraction of about 20% of the amount of C₃A is found to contribute to formation of Friedel's salt. Higher amounts of Friedel's salt are formed in the metakaolin containing mortars. However, the limited chloride ingress depths prevent quantification of the potential full chloride binding capacity of Friedel's salt in these mortars. The measured amounts of Friedel's salt by TGA and the portlandite profiles show that the maximum amount of Friedel's salt is found in the region with limited leaching of calcium, which is in good agreement with the predicted Friedel's salt profiles.

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry, Norwegian University of Science and Technology, Swiss Federal Laboratories for Materials Science and Technology (Empa), Cementir Holding S.p.A., Aarhus University
Authors: Shi, Z. (Ekstern), Geiker, M. R. (Ekstern), Lothenbach, B. (Ekstern), De Weerdt, K. (Ekstern), Garzón, S. F. (Ekstern), Enemark-Rasmussen, K. (Intern), Skibsted, J. (Ekstern)
Number of pages: 11
Pages: 73-83
Publication date: 1 Apr 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Cement and Concrete Composites
Volume: 78
ISSN (Print): 0958-9465
Ratings:
The present study investigates the coal char combustion by a combination of thermochemical and X-ray photoemission spectroscopy (XPS) analyses. Thermoanalytical methods (differential thermogravimetry, differential scanning calorimetry, and temperature-programmed desorption) are used to identify the key reactive steps that occur upon oxidation and...
heating of coal char (chemisorption, structural rearrangement and switchover of surface oxides, and desorption) and their energetics. XPS is used to reveal the chemical nature of the surface oxides that populate the char surface and to monitor their evolution throughout thermochemical processing. XPS spectra show the presence on the carbon surface of three main components. It is shown that the most abundant oxygen functionality in the raw char is epoxy. It decreases with preoxidation at 300°C and even more at 500°C, where carboxyl and ether oxygen functionalities prevail. The rearrangement of epoxy during preoxidation goes together with activation of the more stable and less reactive carbon sites. Results are in good agreement with semi-lumped kinetic models of carbon oxidation, which include (1) formation of "metastable" surface oxides, (2) complex switchover, and (3) desorption into CO and CO₂.

**General information**

**State:** Published

**Organisations:** Department of Chemistry, Sincrotrone Trieste, CNR, University of Naples Federico II

**Authors:** Levi, G. (Intern), Causà, M. (Ekstern), Lacovig, P. (Ekstern), Salatino, P. (Ekstern), Senneca, O. (Ekstern)

**Number of pages:** 9

**Pages:** 2308-2316

**Publication date:** 16 Mar 2017

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

**Publication information**

**Journal:** Energy and Fuels

**Volume:** 31

**Issue number:** 3

**ISSN (Print):** 0887-0624

**Ratings:**

- BFI (2018): BFI-level 2
- Web of Science (2018): Indexed yes
- BFI (2017): BFI-level 2
- Web of Science (2017): Indexed yes
- BFI (2016): BFI-level 2
- Scopus rating (2016): CiteScore 3.49
- Web of Science (2016): Indexed yes
- BFI (2015): BFI-level 2
- Scopus rating (2015): CiteScore 3.34
- Web of Science (2015): Indexed yes
- BFI (2014): BFI-level 2
- Scopus rating (2014): CiteScore 3.3
- Web of Science (2014): Indexed yes
- BFI (2013): BFI-level 2
- Scopus rating (2013): CiteScore 3.52
- ISI indexed (2013): ISI indexed yes
- Web of Science (2013): Indexed yes
- BFI (2012): BFI-level 2
- Scopus rating (2012): CiteScore 3.25
- ISI indexed (2012): ISI indexed yes
- Web of Science (2012): Indexed yes
- BFI (2011): BFI-level 2
- Scopus rating (2011): CiteScore 3.05
- ISI indexed (2011): ISI indexed yes
- Web of Science (2011): Indexed yes
- BFI (2010): BFI-level 2
- Web of Science (2010): Indexed yes
- BFI (2009): BFI-level 2
- Web of Science (2009): Indexed yes
- BFI (2008): BFI-level 2
- Web of Science (2008): Indexed yes
- Web of Science (2007): Indexed yes
- Web of Science (2006): Indexed yes
- Web of Science (2005): Indexed yes
Lubrication synergy: Mixture of hyaluronan and dipalmitoylphosphatidylcholine (DPPC) vesicles

Phospholipids and hyaluronan have been implied to fulfill important roles in synovial joint lubrication. Since both components are present in synovial fluid, self-assembly structures formed by them should also be present. We demonstrate by small angle X-ray scattering that hyaluronan associates with the outer shell of dipalmitoylphosphatidylcholine (DPPC) vesicles in bulk solution. Further, we follow adsorption to silica from mixed hyaluronan/DPPC vesicle solution by Quartz Crystal Microbalance with Dissipation measurements. Atomic Force Microscope imaging visualises the adsorbed layer structure consisting of non-homogeneous phospholipid bilayer with hyaluronan/DPPC aggregates on top. The presence of these aggregates generates a long-range repulsive surface force as two such surfaces are brought together. However, the aggregates are easily deformed, partly rearranged into multilayer structures and partly removed from between the surfaces under high loads. These layers offer very low friction coefficient (<0.01), high load bearing capacity (≈23 MPa), and self-healing ability. Surface bound DPPC/hyaluronan aggregates provide a means for accumulation of lubricating DPPC molecules on sliding surfaces.
Effect of solvent quality and chain density on normal and frictional forces between electrostatically anchored thermoresponsive diblock copolymer layers

Equilibration in adsorbing polymer systems can be very slow, leading to different physical properties at a given condition depending on the pathway that was used to reach this state. Here we explore this phenomenon using a diblock copolymer consisting of a cationic anchor block and a thermoresponsive block of poly(2-isopropyl-2-oxazoline), PIPOZ. We find that at a given temperature different polymer chain densities at the silica surface are achieved depending on the previous temperature history. We explore how this affects surface and friction forces between such layers using the atomic force microscope colloidal probe technique. The surface forces are purely repulsive at temperatures <40 °C. A local force minimum at short separation develops at 40 °C and a strong attraction due to capillary condensation of a polymer-rich phase is observed close to the bulk phase separation temperature. The friction forces decrease in the cooling stage due to rehydration of the PIPOZ chain. A consequence of the adsorption hysteresis is that the friction forces measured at 25 °C are significantly lower after exposure to a temperature of 40 °C than prior to heating, which is due to higher polymer chain density on the surface after heating.

General information
A windshield washer concentrate and the use thereof
The present invention relates to a windshield washer concentrate comprising a first compound and alcohol, wherein said first compound is ammonium acetate or ammonium formate or a combination thereof, and wherein the concentrate comprises the first compound in an amount of at least 5g per litre alcohol.

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry
Authors: Kegnæs, S. (Intern), Hansen, C. L. (Ekstern), Le Quement, S. T. (Ekstern)
Publication date: 19 Jan 2017

Publication information
IPC: C11D 7/26 A I
Patent number: WO2017008810
Date: 19/01/2017
Priority date: 10/07/2015
Priority number: EP20150176262
Original language: English
Electronic versions:
WO2017008810A1.pdf
Main Research Area: Technical/natural sciences
Source: espacenet
Source-ID: WO2017008810
Publication: Research › Patent – Annual report year: 2017

PROCESS FOR HYDROGENOLYSIS OF ALPHA-HYDROXY ESTERS OR ACIDS USING A HETEROGENEOUS CATALYST
The present invention relates to a method for hydrogenolysis of alpha-hydroxy esters or acids, comprising reacting the alpha-hydroxy ester or acid in the presence of a heterogeneous catalyst. The present invention also relates to a method for producing propionic acid ester, and the use of any of the methods for the production of propionic acid esters, such as alkyl propionate.

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry
Authors: Saravanamurugan, S. (Intern), Khokarale, S. G. (Intern), Riisager, A. (Intern)
Publication date: 5 Jan 2017

Publication information
IPC: C07C 67/327 A I
Patent number: WO2017001285

17th International Conference on Petroleum Phase Behavior and Fouling

This special section of Energy & Fuels contains contributed papers from the 17th International Conference on Petroleum Phase Behavior and Fouling (Petrophase 2016). Petrophase 2016 was organized by the Technical University of Denmark and Schlumberger and took place in Elsinore (Helsingør) Denmark from June 19th to 23rd at the Beach Hotel Marienlyst. Petrophase is an international conference aimed at researchers in industry and academia dedicated to the study of the properties and chemistry of petroleum fluids and their effect on producing, processing, and refining in the upstream, midstream, and downstream industries. The conference started in 1999 as “The International Conference on Petroleum Phase Behavior & Fouling” and has since evolved into an annual event taking place in countries all around the world. Petrophase has been fortunate to have enjoyed financial and organizational support from many academic and industrial institutions through the years. Despite its growth over the years, Petrophase has always had the feel of an intimate conference where all participants are present in all of the activities.

General information
State: Published
Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, Department of Chemistry, Asphalteam
Authors: von Solms, N. (Intern), Yan, W. (Intern), Andersen, S. (Ekstern)
Pages: 3329-3329
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Energy and Fuels
Volume: 31
Issue number: 4
ISSN (Print): 0887-0624
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.49
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 3.34
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 3.3
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 3.52
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 3.25
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Ab Initio Assessment of the Bonding in Disulfonates Containing Divalent Nitrogen and Phosphorus Atoms

The iminodisulfonate, \([\text{N(SO}_3\text{)}_2]^{3-}\), and phosphinodisulfonate, \([\text{P(SO}_3\text{)}_2]^{3-}\), ions have been investigated by performing ab initio MP2/6-311+G** calculations. The nitrogen and phosphorus atoms as part of the ions are shown to be divalent with a negative charge and two lone pairs on the nitrogen and phosphorus atoms. The experimentally known calcium sodium iminodisulfonate trihydrate and the analogous unknown compound calcium sodium phosphinodisulfonate trihydrate have also been investigated using the MP2/6-311+G** calculations. For the nitrogen compound, only minor changes occur in the iminodisulfonate ion when it becomes part of the calcium sodium iminodisulfonate trihydrate. For the phosphorus compound, the geometry of the phosphinodisulfonate ion changes significantly as part of calcium sodium phosphinodisulfonate trihydrate. Furthermore, the charges associated with the atoms in calcium sodium phosphinodisulfonate trihydrate are quite different from those of the phosphinodisulfonate ion. For calcium sodium iminodisulfonate trihydrate, the Raman spectrum has been measured, and it compares well with the spectrum derived using HF/6-311+G** calculations.
A broad range quorum sensing inhibitor working through sRNA inhibition

For the last decade, chemical control of bacterial virulence has received considerable attention. Ajoene, a sulfur-rich molecule from garlic has been shown to reduce expression of key quorum sensing regulated virulence factors in the opportunistic pathogen *Pseudomonas aeruginosa*. Here we show that the repressing effect of ajoene on quorum sensing occurs by inhibition of small regulatory RNAs (sRNA) in *P. aeruginosa* as well as in *Staphylococcus aureus*, another important human pathogen that employs quorum sensing to control virulence gene expression. Using various reporter constructs, we found that ajoene lowered expression of the sRNAs RsmY and RsmZ in *P. aeruginosa* and the small dual-function regulatory RNA, RNAIII in *S. aureus*, that controls expression of key virulence factors. We confirmed the modulation of RNAIII by RNA sequencing and found that the expression of many QS regulated genes encoding virulence factors such as hemolysins and proteases were lowered in the presence of ajoene in *S. aureus*. Importantly, our findings show that sRNAs across bacterial species potentially may qualify as targets of anti-virulence therapy and that ajoene could be a lead structure in search of broad-spectrum compounds transcending the Gram negative-positive borderline.
Accessing Tri-substituted γ-Lactam Scaffolds Via Cascade Reactions: What Opportunities For Libraries!

The European Lead Factory is an EU-based initiative (part of the Innovative Medicines Initiative), which has been set to foster drug discovery in Europe. Among the objectives, a 200,000-compound collection is being generated. Lactams represent a large class of valuable scaffolds for medicinal chemistry and remain a wide and interesting area of study. In this context, 2 libraries based on a 1,4,5 γ-lactam core have been designed and produced using cascade reactions involving an aldehyde moiety, an amine and a nucleophilic partner as the key reaction. One library is focused on a 3-MCR on oxo-esters, while the other is based on a Ritter-type cascade. On several occasions these multi-component and one-pot processes have been used directly as the production step, thus allowing very fast and diverse library syntheses, whereas in other cases, the choice of partners bearing other anchoring groups permitted further functionalization and the production of even more diverse members of the libraries. The > 1,000 compounds based on these scaffolds have been delivered for HTS at the European Screening Center where they are currently being tested.

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry, EDELRIS
Authors: Bonnet, K. (Ekstern), Clausen, M. H. (Intern), Fleury-Brégeot, N. (Ekstern), Lardy, C. (Ekstern), Morgentin, R. (Ekstern), Nielsen, T. E. (Intern), Petersen, M. Å. (Intern), Rasmussen, M. O. (Ekstern), Roche, D. (Ekstern), Wu, P. (Intern)
Publication date: 2017
Conference: Experimental Biology 2016 Meeting, San Diego, United States, 02/04/2016 - 02/04/2016
Main Research Area: Technical/natural sciences

Publication information
Journal: F A S E B Journal
Volume: 30
Issue number: 1
ISSN (Print): 0892-6638
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.68 SJR 2.57 SNIP 1.22
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 2.788 SNIP 1.249 CiteScore 4.68
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.993 SNIP 1.342 CiteScore 4.92
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 3.116 SNIP 1.4 CiteScore 5.5
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 3.071 SNIP 1.441 CiteScore 5.6
ISI indexed (2012): ISI indexed yes
A Dereplication and Bioguided Discovery Approach to Reveal New Compounds from a Marine-Derived Fungus Stilbella fimetaria

A marine-derived Stilbella fimetaria fungal strain was screened for new bioactive compounds based on two different approaches: (i) bio-guided approach using cytotoxicity and antimicrobial bioassays; and (ii) dereplication based approach using liquid chromatography with both diode array detection and high resolution mass spectrometry. This led to the discovery of several bioactive compound families with different biosynthetic origins, including pimarane-type diterpenoids and hybrid polyketide-non ribosomal peptide derived compounds. Prefractionation before bioassay screening proved to be a great aid in the dereplication process, since separate fractions displaying different bioactivities allowed a quick tentative identification of known antimicrobial compounds and of potential new analogues. A new pimarane-type diterpene, myrocin F, was discovered in trace amounts and displayed cytotoxicity towards various cancer cell lines. Further media optimization led to increased production followed by the purification and bioactivity screening of several new and known pimarane-type diterpenoids. A known broad-spectrum antifungal compound, ilicicolin H, was purified along with two new analogues, hydroxyl-ilicicolin H and ilicicolin I, and their antifungal activity was evaluated.

General information
State: Published
Organisations: Department of Biotechnology and Biomedicine, Natural Product Discovery, Department of Chemistry, Organic Chemistry, Fungal Degradation, Fungal Chemodiversity, German Cancer Research Center (DKFZ), Fundación MEDINA
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Marine Drugs
Volume: 15
Issue number: 8
Article number: 253
ISSN (Print): 1660-3397
A Linker for the Solid-Phase Synthesis of Hydroxamic Acids and Identification of HDAC6 Inhibitors

We herein present broadly useful, readily available and nonintegral hydroxylamine linkers for the routine solid-phase synthesis of hydroxamic acids. The developed protocols enable the efficient synthesis and release of a wide range of hydroxamic acids from various resins, relying on high control and flexibility with respect to reagents and synthetic processes. A trityl-based hydroxylamine linker was used to synthesize a library of peptide hydroxamic acids. The inhibitory effects of the compounds were examined for seven HDAC enzyme subtypes using a chemiluminescence-based assay.

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry, University of Copenhagen, Nanyang Technological University
HDAC inhibitor, Hydroxamic acid, Linker, Solid-phase synthesis

DOIs:
10.1021/acscombsci.7b00068

Source: FindIt
Alzheimer's disease: How metal ions define β-amyloid function

Alzheimer’s disease is increasingly recognized to be linked to the function and status of metal ions, and recently, the amyloid hypothesis has been strongly intertwined with the metal ion hypothesis; in fact, these two hypotheses fit well together and are not mutually contradictory. This review focuses on the essential coordination chemistry and biochemistry that relate transition metal ions iron, copper, and zinc to β-amyloid (Aβ) and most likely define the peptide’s roles in neurons. The metal-Aβ interactions have elements of both gain of toxic function, as usually considered, but also loss of natural functions, as emphasized in this review. Both these aspects and their relationships are discussed and their implications for future therapeutic strategies are outlined.

General information
State: Published
Organisations: Department of Chemistry
Authors: Kepp, K. P. (Intern)
Pages: 127-159
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Coordination Chemistry Reviews
Volume: 351
ISSN (Print): 0010-8545
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 11.43 SJR 4.164 SNIP 3.021
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 3.957 SNIP 3.281 CiteScore 12.29
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 4.551 SNIP 3.444 CiteScore 11.85
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 4.366 SNIP 3.651 CiteScore 11.53
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 5.039 SNIP 3.782 CiteScore 11.6
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 4.525 SNIP 3.85 CiteScore 11.11
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 4.557 SNIP 3.467
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 5.104 SNIP 3.661
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2007): SJR 5.128 SNIP 3.909
Scopus rating (2006): SJR 4.118 SNIP 3.856
Scopus rating (2005): SJR 4.056 SNIP 3.379
Scopus rating (2004): SJR 2.988 SNIP 2.963
An efficient synthesis of linear β-(1→6)-galactan oligosaccharides related to plant cell wall glycans

Galactans are linear structures mainly found in arabinogalactan glycans and RG-I side chains. As a follow-up to our work on both β-(1→3)-linked and β-(1→4)-linked galactans, we herein report a convergent synthesis of β-(1→6)-galactan using our previously synthesized 4,6-benzylidene protected disaccharide as a key building block. However, the regioselective reductive opening of the 4,6-benzylidene protected disaccharide turned out to become more challenging as the length of the oligosaccharide increased and a second differential protected disaccharide building block carrying a chloroacetyl group on the 6-position was used to elongate the chain in a more efficient way.

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry
Authors: Andersen, M. C. F. (Intern), Arentoft, C. A. S. (Intern), Boos, I. (Intern), Kinnaert, C. (Intern), Awan, S. I. (Intern), Clausen, M. H. (Intern)
Pages: 27-37
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Trends in Carbohydrate Research
Volume: 9
Issue number: 2
ISSN (Print): 0975-0304
Ratings:
Web of Science (2018): Indexed yes
Web of Science (2017): Indexed yes
Scopus rating (2016): SJR 0.15 SNIP 0.057
Scopus rating (2015): SJR 0.124 SNIP 0.067
Scopus rating (2014): SJR 0.157 SNIP 0.164
Scopus rating (2013): SJR 0.139 SNIP 0.136
Scopus rating (2012): SJR 0.145 SNIP 0.203
Scopus rating (2011): SJR 0.121 SNIP 0.081
Scopus rating (2010): SJR 0.189 SNIP 0.13
Original language: English
Plant cell wall oligosaccharides, Arabinogalactans, RG-I, β-(1→6)-D-galactans

A Novel Model on DST-Induced Transplantation Tolerance by the Transfer of Self-Specific Donor iTregs to a Haploype-Matched Organ Recipient

Donor-specific blood transfusion (DST) can lead to significant prolongation of allograft survival in experimental animal models and sometimes human recipients of solid organs. The mechanisms responsible for the beneficial effect on graft survival have been a topic of research and debate for decades and are not yet fully elucidated. Once we discover how the details of the mechanisms involved are linked, we could be within reach of a procedure making it possible to establish donor-specific tolerance with minimal or no immunosuppressive medication. Today, it is well established that CD4+Foxp3+ regulatory T cells (Tregs) are indispensable for maintaining immunological self-tolerance. A large number of animal studies have also shown that Tregs are essential for establishing and maintaining transplantation tolerance. In this paper, we present a hypothesis of one H2-haplotype-matched DST-induced transplantation tolerance (in mice). The formulated hypothesis is based on a re-interpretation of data from an immunogenetic experiment published by Niimi and colleagues in 2000. It is of importance that the naive recipient mice in this study were never immunosuppressed and were therefore fully
immune competent during the course of tolerance induction. Based on the immunological status of the recipients, we suggest that one H2-haplotype-matched self-specific Tregs derived from the transfusion blood can be activated and multiply in the host by binding to antigen-presenting cells presenting allopeptides in their major histocompatibility complex (MHC) class II (MHC-II). We also suggest that the endothelial and epithelial cells within the solid organ allograft upregulate the expression of MHC-II and attract the expanded Treg population to suppress inflammation within the graft. We further suggest that this biological process, here termed MHC-II recruitment, is a vital survival mechanism for organs (or the organism in general) when attacked by an immune system.

General information
State: Published
Organisations: Department of Chemistry, University of Copenhagen
Authors: Gregoriussen, A. M. M. (Ekstern), Bohr, H. G. (Intern)
Pages: 1-9
Publication date: 2017
Main Research Area: Technical/natural sciences

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A Pd-Catalyzed in situ domino process for mild and quantitative production of 2,5-dimethylfuran directly from carbohydrates
An in situ domino process has been developed to be highly efficient for direct and mild conversion of various hexose sugars to the biofuel 2,5-dimethylfuran in almost quantitative yields, without separation of unstable intermediates at 120 °C in n-butanol, by using polymethylhydrosiloxane and hydrophobic Pd/C as a H-donor and a bifunctional catalyst, respectively. Among the cascade reactions, the hydrosilylation process was confirmed by deuterium-labeling and kinetic studies to be favorable for sugar dehydration and exclusively acts on deoxygenation of in situ formed intermediates including furanic alcohols and aldehydes to DMF via a hydride transfer process that was facilitated by an alcoholic solvent. The catalytic system is more selective than the H2-participated counterpart, and could be scaled up with only 0.04 mol% catalyst loading, giving DMF in a comparable yield of 85%. Moreover, Pd(0) was demonstrated to be the active species for deoxygenation, and the heterogeneous catalyst exhibited good recyclability with little elemental leaching.

General information
Application of a Crossover Equation of State to Describe Phase Equilibrium and Critical Properties of n-Alkanes and Methane/n-Alkane Mixtures

Crossover equations of state (EOSs) are models that incorporate density fluctuations into mean-field thermodynamic models, changing their behavior close to the critical point. In this way, they are capable of describing the analytical behavior of fluids far from the critical region and the asymptotic one near the critical point. Although several crossover EOSs have been developed in the last decades, their use in modeling industrial processes is rather limited. In this work, we use the crossover Soave–Redlich–Kwong (CSRK) to describe phase equilibrium and critical properties of pure n-alkanes and methane/n-alkane binary mixtures and compare the results to two other modeling approaches of the SRK EOS. In the case of the pure fluids, CSRK gives an accurate overall description of the phase equilibrium and critical properties; nevertheless, a minor increase in the deviation of the saturation pressure and other properties is observed when compared to that of the mean-field model. For the binary mixtures, an improvement in the description of the critical volumes is seen, while, for the other properties, similar results are obtained.

General information
State: Accepted/In press
Organisations: Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources, Engineering, Department of Chemistry, KT Consortium
Authors: P. C. M. Vinhal, A. (Intern), Yan, W. (Intern), Kontogeorgis, G. M. (Intern)
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Scopus rating (2016): CiteScore 2.29 SJR 0.88 SNIP 1.097
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Scopus rating (2014): SJR 1.021 SNIP 1.208 CiteScore 2.22
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ISI indexed (2013): ISI indexed yes
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BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.141 SNIP 1.103 CiteScore 2.01
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.862 SNIP 0.988 CiteScore 1.8
Application of Iterative Robust Model-based Optimal Experimental Design for the Calibration of Biocatalytic Models

The aim of model calibration is to estimate unique parameter values from available experimental data, here applied to a biocatalytic process. The traditional approach of first gathering data followed by performing a model calibration is inefficient, since the information gathered during experimentation is not actively used to optimise the experimental design. By applying an iterative robust model-based optimal experimental design, the limited amount of data collected is used to design additional informative experiments. The algorithm is used here to calibrate the initial reaction rate of an ω-transaminase catalysed reaction in a more accurate way. The parameter confidence region estimated from the Fisher Information Matrix is compared with the likelihood confidence region, which is more accurate, but also more expensive. As a result, an important deviation between both approaches is found, confirming that linearisation methods should be applied with care for nonlinear models. This article is protected by copyright. All rights reserved.

General information
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Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Department of Chemistry, Ghent University, Lund University
Pages: 1278–1293
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Journal: Biotechnology Progress
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Applying fluorescence correlation spectroscopy to investigate peptide-induced membrane disruption

There is considerable interest in understanding the interactions of antimicrobial peptides with phospholipid membranes. Fluorescence correlation spectroscopy (FCS) is a powerful experimental technique that can be used to gain insight into these interactions. Specifically, FCS can be used to quantify leakage of fluorescent molecules of different sizes from large unilamellar lipid vesicles, thereby providing a tool for estimating the size of peptide-induced membrane disruptions. If fluorescently labeled lipids are incorporated into the membranes of the vesicles, FCS can also be used to obtain information about whether leakage occurs due to localized membrane perturbations or global membrane destabilization. Here, we outline a detailed step-by-step protocol on how to optimally implement an FCS-based leakage assay. To make the protocol easily accessible to other researchers, it has been supplemented with a number of practical tips and tricks.

General information
State: Published
Organisations: Department of Micro- and Nanotechnology, Colloids and Biological Interfaces, Center for Nanomedicine and Theranostics, Department of Chemistry
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A straight forward approach to electrodeposit tungsten disulfide/poly(3,4-ethylenedioxythiophene) composites onto nanoporous gold for the hydrogen evolution reaction

1.1nm tungsten disulfide/poly(3,4-ethylenedioxythiophene) (PEDOT) was successfully electrodeposited on the surface of dealloyed nanoporous gold (NPG) surface to form uniform nanocomposites and offers an excellent electrocatalysis for the electrochemical dihydrogen evolution reaction (HER) in acidic media. The approach is straight forward and does not require any expensive equipment or intensive energy. The morphology and composition of the nanocomposites were structurally mapped by high-resolution transmission electron microscopy (HRTEM), X-ray photoelectron spectroscopy (XPS) and Fourier transform infrared spectrometry (FTIR). The roles of both the NPG substrate and PEDOT in the observed enhanced HER activity compared to planar Au-electrode surfaces and pure single-component WS2 have been deconvoluted experimentally. PEDOT itself is inert for the HER, but was found to improve significantly the conductivity and operating stability of the WS2 catalyst. The prepared nanocomposites reach the best in 2D WS2 catalyst family, exhibiting excellent electrochemical catalytic activity for the HER. The optimal electrode showed an onset potential of -164 mV vs. reversible hydrogen electrode (RHE), an apparent exchange current density as high as 0.04 mAcm-2, and a very low Tafel slope of 53mV dec-1. These catalysts are promising electrocatalysts for generation a large amount of H2 from water.

General information
State: Published
Organisations: Department of Chemistry, NanoChemistry, Organic Chemistry, Shandong University, Aarhus University
Authors: Xiao, X. (Ekstern), Engelbrekt, C. (Intern), Zhang, M. (Intern), Li, Z. (Ekstern), Ulstrup, J. (Intern), Zhang, J. (Intern), Si, P. (Ekstern)
Number of pages: 7
Pages: 308-314
Asymmetric Total Syntheses of (-)-α-Lycorane, (-)-Zephyranthine and Formal Synthesis of (+)-Clivonine

We report the successful achievement of an asymmetric route to (-)-α-lycorane and (-)-zephyranthine as well as a formal total synthesis of (+)-clivonine. A pivotal intermediate, which serves as a potent precursor for the divergent syntheses of these natural products, was accessed by a diastereoselective Pd-catalyzed cinnamylation of an N-tert-butanesulfinyl imine.

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry, Fudan University
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Scopus rating (2014): SJR 1.762 SNIP 0.974 CiteScore 4.38
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Scopus rating (2013): SJR 1.767 SNIP 0.872 CiteScore 4.12
ISI indexed (2013): ISI indexed yes
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Scopus rating (2012): SJR 2.267 SNIP 1.026 CiteScore 4.36
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.31 SNIP 1.017 CiteScore 4.43
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
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A synthetic glycan microarray enables epitope mapping of plant cell wall glycan-directed antibodies

In the last three decades, more than 200 monoclonal antibodies have been raised against most classes of plant cell wall polysaccharides by different laboratories world-wide. These antibodies are widely used to identify differences in plant cell wall components in mutants, organ and tissue types, and developmental stages. Despite their importance and broad use, the precise binding epitope for only a few of these antibodies has been determined. Here, we use a plant glycan microarray equipped with 88 synthetic oligosaccharides to comprehensively map the epitopes of plant cell wall glycan-directed antibodies. Our results reveal the binding epitopes for 78 arabinogalactan-, rhamnogalacturonan-, xylan-, and xyloglucan-directed antibodies. We demonstrate that, with knowledge of the exact epitopes recognized by individual antibodies, specific glycosyl hydrolases can be implemented into immunological cell wall analyses, providing a framework to obtain structural information on plant cell wall glycans with unprecedented molecular precision.

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry, Max Planck Institute of Colloids and Interfaces, Freie Universitat Berlin, Saitama University, University of Leeds, University of Georgia
Authors: Ruprecht, C. (Ekstern), Bartetzko, M. P. (Ekstern), Senf, D. (Ekstern), Dallabernardina, P. (Ekstern), Boos, I. (Intern), Andersen, M. C. F. (Intern), Kotake, T. (Ekstern), Knox, J. P. (Ekstern), Hahn, M. G. (Ekstern), Clausen, M. H. (Intern), Pfrengle, F. (Ekstern)
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Scopus rating (2011): SJR 3.864 SNIP 1.857 CiteScore 6.45
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Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 3.775 SNIP 1.715
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 4.099 SNIP 1.796
Bacterial Electrocatalysis of K₄[Fe(CN)₆] Oxidation

_Shewanella oneidensis_ MR-1 (MR-1), a model strain of electrochemically active bacteria, can transfer electrons from cell to extracellular electron acceptors including Fe(III) (hydro)oxides. It has been reported that several redox species such as cytochromes in membranes and flavins assist in the electron transport (ET) processes. However, the oxidation of metal compounds was barely described. Here we report electrocatalysis of K₄[Fe(CN)₆] oxidation by MR-1. K₄[Fe(CN)₆] is a redox inorganic compound and shows a reversible redox process on bare glassy carbon (GCE). This is reflected by a pair of symmetric peaks on cyclic voltammetry (CV) (Fig. 1). Interestingly, unsymmetric peaks with a strong anodic peak and a very weak cathodic peak are found on CVs of 1.0 mM K₄[Fe(CN)₆] when the GCE was coated with MR-1, distinguished from the reversible CV on bare electrodes (Fig. 1). A similar electrochemical pattern has been observed using K₃[Fe(CN)₆]. These results suggested an electrocatalysis process of [Fe(CN)]₄³⁻ to [Fe(CN)]₃⁺ by MR-1. The ratio of anodic peak current vs cathodic peak current depends on scan rate, suggesting both diffusion of redox molecules and interfacial ET rate are key factors of the electrocatalysis. Moreover, Selectivity of MR-1 is another interesting issue: MR-1 does not catalyze other redox compounds such as Ru[(NH₃)₆]Cl₃ and Resorufin. In our recent work, extracellular polymeric substances (EPS) showed redox properties and electron hopping through EPS. Here we notice that neither the glassy carbon electrode (GCE) coating EPS extracted from MR-1 nor MR-1 removed EPS (MR-1ΔEPS) exhibited asymmetric redox feature (Fig. 1), but caused the decrease of current and the broadening of the difference of anodic and cathodic peak potential, indicating the hindrance of reaction. More work to disclose the origin of the electrocatalysis phenomenon is in progress, aiming at the identification of related compositions in MR-1.

General information
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Organisations: Department of Chemistry, NanoChemistry, Metalloprotein Chemistry and Engineering, Organic Chemistry, Chinese Academy of Sciences
Authors: Zheng, Z. (Intern), Xiao, Y. (Intern), Wu, R. (Intern), Christensen, H. E. M. (Intern), Zhao, F. (Ekstern), Zhang, J. (Intern)
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Barley genotypic β-glucan variation combined with enzymatic modifications direct its potential as a natural ingredient in a high fiber extract

β-Glucan was extracted from eight different barley genotypes varying in β-glucan content and molecular structure using Termamyl® SC (T), Attenuzyme® (A) and Attenuzyme® Flex (AF) amylolytic enzymes in combinations. Extracts from barley lines Lys5f, KVL408, KVL1104 and CDC Fibar exceeded 4 g β-glucan/l, providing European Food Safety Authority (EFSA) and U.S. Food and Drug Administration (FDA) recommended amounts (3 g β-glucan/day) from three portions. TAF extracts of Lys5f and KVL408 grains reached extraordinary high concentrations of 8-9 g β-glucan/l. The β-glucan molecular mass decreased with enzyme treatment T < TA < TAF due to minor lichenase side activity. Extractability was generally higher and molecular mass lower for barley lines low in triosyl/tetraosyl (DP3/DP4) ratios than for those high in DP3/DP4 ratios (Lys5f, KVL408 and KVL1104). Overall, the higher β-glucan content and structural robustness in Lys5f and KVL408 raw materials favor these in a β-glucan rich extract with potential for EFSA and FDA health and Nutrition claims.
Benchmarking Density Functionals for Chemical Bonds of Gold

Gold plays a major role in nanochemistry, catalysis, and electrochemistry. Accordingly, hundreds of studies apply density functionals to study chemical bonding with gold, yet there is no systematic attempt to assess the accuracy of these methods applied to gold. This paper reports a benchmark against 51 experimental bond enthalpies of AuX systems and seven additional polyatomic and cationic molecules. Twelve density functionals were tested, covering meta functionals, hybrids with variable HF exchange, double-hybrid, dispersion-corrected, and nonhybrid GGA functionals. The defined benchmark data set probes all types of bonding to gold from very electronegative halides that force Au+ electronic structure, via covalently bonded systems, hard and soft Lewis acids and bases that either work against or complement the softness of gold, the Au2 molecule probing gold’s bond with itself, and weak bonds between gold and noble gases. Zero-point vibrational corrections are relatively small for Au-X bonds, ~11-12 kJ/mol except for Au-H bonds. Dispersion typically provides ~5 kJ/mol of the total bond enthalpy but grows with system size and is 10 kJ/mol for AuXe and AuKr. HF exchange and LYP correlation produce weaker bonds to gold. Most functionals provide similar trend accuracy, though somewhat lower for M06 and M06L, but very different numerical accuracy. Notably, PBE and TPSS functionals with dispersion display the smallest numerical errors and very small mean signed errors (0-6 kJ/mol), i.e. no bias toward over- or under-binding. Errors are evenly distributed versus atomic number, suggesting that relativistic effects are treated fairly; the mean absolute error is almost halved from B3LYP (45 kJ/mol) to TPSS and PBE (23 kJ/mol, including difficult cases); 23 kJ/mol is quite respectable considering the diverse bonds to gold and the complication of relativistic effects. Thus, studies that use DFT with effective core potentials for gold chemistry, with no alternative due to computational cost, are on solid ground using TPSS-D3 or PBE-D3.

General information
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Organisations: Department of Chemistry
Authors: Kepp, K. P. (Intern)
Pages: 2022-2034
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BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.64
Biocompatible Nanoengineering of Graphene based Materials for Sensor Applications

Personalized healthcare and diagnostics is one of the most active areas of research in both academia and industry. Point-of-care sensing devices for monitoring and regulating from simple ions to large complex molecules are essential in our everyday life. These simple and inexpensive devices permit an individual to perform urgent diagnostic analyses without the need of a professional training or expensive laboratory facilities. Application of these point-of-care sensing devices has the potential to revolutionize the healthcare sectors particularly in developing countries with limited access to modern high tech facilities or in other sectors such as food safety control, forensics and environmental monitoring. Nanomaterials are very promising for the development of these sensing devices. Graphene, an atomically thick layer of graphite, is considered as one of the most fascinating nanomaterials due to its unique physicochemical properties and versatile application potential. The aim of this PhD project is to develop graphene based low cost point-of-care electrochemical sensing devices for a broad range of applications. To maintain the low-cost profile and reduce environmental footprint, we have demonstrated the biocompatible nanoengineering of graphene, which is nanoscale functionalization to improve its biocompatibility, stability and ease of processability for the development of chemosensing and biosensing platforms. The first graphene based chemosensing application was graphene biofunctionalized with the small biomolecule dopamine and was used for melamine detection. In the next step, twenty different amino acids were used for the green synthesis of nitrogen doped graphene. Among all twenty amino acids, lysine was found as the most efficient one and the resulting nitrogen-doped graphene was used for dopamine chemosensing. For other graphene based biosensing applications, graphene was first functionalized with a branched polymer to derive a biocompatible graphene matrix for stable
accommodation of more complex bio-recognition element such as enzymes. The biocompatible engineered graphene was
used for novel glucose biosensing. In the next step, the pre-synthesized biocompatible graphene was functionalized with a
redox active molecule, ferrocene. The as synthesized redox active and biocompatible graphene was further functionalized
with enzymes and used for glucose and cholesterol biosensing. Finally, the bio-functionalized graphene was step wisely
converted to aprintable ink and further used for fabrication of flexible and screen-printdbiosensing devices. The screen
printed electrodes were tested for the glucose level measurements in real human serum samples, and found to be closely
comparable with the results obtained by the standard clinical methods in a hospital.

General information
State: Published
Organisations: Department of Chemistry, NanoChemistry, Organic Chemistry
Authors: Halder, A. (Intern), Chi, Q. (Intern), Ulstrup, J. (Intern)
Number of pages: 180
Publication date: 2017

Bioenergy conversion and storage systems: from conventional electrochemical cells to hybrid bioelectronic devices
The rapid development and popularization of wearable and implantable self-sustainable electronics has increasingly
demanded new-generation miniature and biocompatible power systems that can function under near-neutral pH solution
and ambient conditions. Towards this end, enzymatic fuel cells (EFCs) using biocatalysts can offer an effective alternative
to conventional batteries or fuel cells attributed to high biocatalytic activity, substrate specified selectivity, and non-toxic
end products with ecofriendly impacts. Newly emerging photobioelectrochemical cells (PBCs), exploiting photosynthetic
machinery for direct conversion of solar energy into electric power, is one of the most promising prospects for green and
selfsustainable energy harvesting. In addition, utilizing the inherent capacitance of electrodes as an activecharge-storing
element enables to enhance the efficiency of electron transfer processes proceeding in the system and further
miniaturization and simplification of a full-function device by elimination of internal capacitors in the electronic circuit.
Remarkably, some pioneering attempts to design and create hybrid bioelectrochemical cells have already shown the
positive prospects of such an approach, which was not able to achieve previously. This invited talk aims to overview
recent developments of EFCs and PBCs. In particular, we highlight their advantages, drawbacks and future perspectives
towards practical applications.

General information
State: Published
Organisations: Department of Chemistry, NanoChemistry, Organic Chemistry
Authors: Pankratov, D. (Intern), Chi, Q. (Intern)
Number of pages: 1
Publication date: 2017

Branched pectic galactan in phloem-sieve-element cell walls: implications for cell mechanics
A major question in plant biology concerns the specification and functional differentiation of cell types. This is in the
context of constraints imposed by networks of cell walls that both adhere cells and contribute to the form and function of
developing organs. Here, we report the identification of a glycan epitope that is specific to phloem sieve element cell walls
in several systems. A monoclonal antibody, designated LM26, binds to the cell wall of phloem sieve elements in stems of
Arabidopsis thaliana, Miscanthus x giganteus and notably sugar beet (Beta vulgaris) roots where phloem identification is
an important factor for the study of phloem unloading of sucrose. Using microarrays of synthetic oligosaccharides, the
LM26 epitope has been identified as a β-1,6-galactosyl substitution of β-1,4-galactan requiring more than three backbone residues for optimized recognition. This branched galactan structure has previously been identified in garlic bulbs in which the LM26 epitope is widespread throughout most cell walls including those of phloem cells. Garlic bulb cell wall material has been used to confirm the association of the LM26 epitope with cell wall pectic rhamnogalacturonan-I (RG-I) polysaccharides. In the phloem tissues of grass stems, the LM26 epitope has a complementary pattern to that of the LM5 linear β-1,4-galactan epitope which is detected only in companion cell walls. Mechanical probing of transverse sections of M. x giganteus stems and leaves by atomic force microscopy indicates that phloem sieve element cell walls have a lower indentation modulus (indicative of higher elasticity) than companion cell walls.
Calculation of Multiphase Chemical Equilibrium by the Modified RAND Method

A robust and efficient algorithm for simultaneous chemical and phase equilibrium calculations is proposed. It combines two individual nonstoichiometric solving procedures: a nested-loop method with successive substitution for the first steps and final convergence with the second-order modified RAND method. The modified RAND extends the classical RAND method from single-phase chemical reaction equilibrium of ideal systems to multiphase chemical equilibrium of nonideal systems. All components in all phases are treated in the same manner and the system Gibbs energy can be used to monitor convergence. This is the first time that modified RAND was applied to multiphase chemical equilibrium systems. The combined algorithm was tested using nine examples covering vapor–liquid (VLE) and vapor–liquid–liquid equilibria (VLLE) of ideal and nonideal reaction systems. Successive substitution provided good initial estimates for the accelerated computation with modified RAND, to ultimately converge to the equilibrium solution without failure.

General information

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Organisations: Department of Chemistry, CERE – Center for Energy Resources Engineering, Technical University of Denmark
Authors: Tsanas, C. (Ekstern), Stenby, E. H. (Intern), Yan, W. (Intern)
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BFI (2015): BFI-level 2
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Web of Science (2015): Indexed yes
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Scopus rating (2014): SJR 1.012 SNIP 1.292 CiteScore 2.85
Web of Science (2014): Indexed yes
Calculation of simultaneous chemical and phase equilibrium by the method of Lagrange multipliers

The purpose of this work is to develop a general, reliable and efficient algorithm, which is able to deal with multiple reactions in multiphase systems. We selected the method of Lagrange multipliers to minimize the Gibbs energy of the system, under material balance constraints. Lagrange multipliers and phase amounts are the independent variables, whose initialization is performed by solving a subset of the working equations. This initialization is the unconstrained minimization of a convex function and it is bound to converge. The whole solution procedure employs a nested loop with Newton iteration in the inner loop and non-ideality updated in the outer loop, thus giving an overall linear convergence rate. Stability analysis is used to introduce additional phases sequentially so as to obtain the final multiphase solution. The procedure was successfully tested on vapor-liquid equilibrium (VLE) and vapor-liquid-liquid equilibrium (VLLE) of reaction systems.
Can Polynuclear Metal Clusters Behave as "Extended" Organometallic Complexes?

Carbon-Increasing Catalytic Strategies for Upgrading Biomass into Energy-Intensive Fuels and Chemicals

Lignocellulosic biomass is the most abundant organic carbon source and has received a great deal of interest as renewable and sustainable feedstock for the production of potential biofuels and value-added chemicals with a wide range of designed catalytic systems. However, those natural polymeric materials are composed of short-chain monomers (typically C6 and C5 sugars) and complex lignin molecules containing plenty of oxygen, resulting in products during the downstream processing having low-grade fuel properties or limited applications in organic syntheses. Accordingly, approaches to increase the carbon-chain length or carbon atom number have been developed as crucial catalytic routes for upgrading biomass into energy-intensive fuels and chemicals. The primary focus of this review is to systematically describe the recent examples on the selective synthesis of long-chain oxygenates via different C-C coupling catalytic processes, such as Aldol condensation, hydroalkylation/alcoholysis, oligomerization, ketonization, Diels-Alder, Guerbet and acylation reactions. Other integrated reaction steps including e.g., hydrolysis, dehydration, oxidation, partial hydrogenation and hydrodeoxygenation (HDO) to derive corresponding key intermediates or final products are also reviewed. The effects of catalyst structure/texture and reaction parameters on the catalytic performance along with relevant reaction mechanisms are in detail discussed. Apart from this, the formation of other useful compounds containing C-X bonds (X = O, N and S) derived from biomass-based substrates for producing fuel additives and valuable chemicals is also briefly reviewed.
Catalytic Oxidation of Allylic Alcohols to Methyl Esters

Aerobic oxidation of allylic alcohols to methyl esters using gold nanoparticles supported on different metal oxide carriers has been performed successfully under mild conditions (room temperature, 0.1 MPa O2) without significant loss of catalytic activity. The effects of different reaction parameters are studied to find the suitable reaction conditions. All catalysts are characterised by XRD, XRF and TEM. Among these catalysts, Au/TiO2 showed the most efficient catalytic activity towards the selective oxidation of allylic alcohols to the corresponding esters. Moreover, the same Au/TiO2 catalyst is used to optimize all the reaction parameters including the significance of the base to promote the reaction. Due to the mild reaction conditions and high conversions as well as selectivity, the utilization of titania-supported gold nanoparticle catalysts represents a benign reaction protocol to synthesize methyl esters from allylic alcohols.
Catalytic Transfer Hydrogenation of Furfural to Furfuryl Alcohol with Recyclable Al-Zr@Fe Mixed Oxides

A series of magnetic, acid/base bifunctional Al–Zr@Fe₃O₄ catalysts were successfully prepared by a facile coprecipitation method and utilized in the catalytic transfer hydrogenation (CTH) of furfural to furfuryl alcohol with 2-propanol as hydrogen source. The physicochemical properties and morphologies of the as-prepared catalysts were characterized by various techniques, including XRD analysis, N₂ physisorption, vibrating sample magnetometry, thermal gravimetry analysis, X-ray fluorescence spectroscopy, NH₃/CO₂ temperature-programmed desorption, SEM, and TEM. The Al₇Zr₃@Fe₃O₄ (1/1) catalyst with a Al³⁺/Zr⁴⁺:Fe³O₄ molar ratio of 21:9:3 was found to exhibit a high furfuryl alcohol yield of 90.5% in the CTH from furfural at 180 °C after 4 h with a comparatively low activation energy of 45.3 kJ mol⁻¹, as calculated from the Arrhenius equation. Moreover, leaching and recyclability tests confirmed Al₇Zr₃@Fe₃O₄ (1/1) to function as a heterogeneous catalyst that could be reused for at least five consecutive reaction runs without significant loss of catalytic activity after simple recovery by an external magnet. Notably, the catalyst proved also efficient for hydrogenation of other biomass-derived furanic aldehydes.

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Challenges and Possibilities of EIS on PEMEC

Electrochemical impedance spectroscopy (EIS) has been proven a very strong electrochemical characterization tool in electrochemical research in general and in the areas of fuel cell and battery research in particular. However, this is not the case for polymer electrolyte membrane electrolysis cells (PEMEC), for which relatively few reports on the application of systematic EIS studies are available. Asking experienced researchers in the field about why, the answer has often been that these cells reveals too much electrical noise to obtain EIS with acceptable quality due to O₂ and H₂ bubble formation. Our view of the ideal structure of a PEMEC is that there ought not to be any effect of gas bubbles on the EIS as the current paths should not be disturbed by bubbles. However, we also see noise in our spectra, but the level of noise varies very much from one cell type to another. We have studied noise on three types of PEMEC and two type of alkaline electrolysis cell (AEC) for comparison. A characteristic feature of the studied PEMEC is that there is no or very little noise seen in the EIS in the frequency range above ca. 500 Hz and again not much noise below 5 Hz. Our hypothesis is that this phenomenon is related to bubbles that are adhering to active sites of the electrocatalyst. When the catalyst layer is subjected to alternating current (AC) during the EIS then, in the PEMEC case, the O₂ pressure and volume of the bubbles growing on the catalyst layer will oscillate with the frequency of the AC. The volume change will naturally change with the frequency. The longer the wave period (the lower the frequency) is, the bigger is the change in the amount of O₂ production during an AC period. In other words, a vibration of the O₂ bubble size and internal pressure must be induced by the AC current. Thus, we imagine that at some low frequency, the bubbles adhering to the catalytic layer get more unstable and detach with an uneven rate from the catalyst surface. This causes the noise observed. Presumably, the structure and the properties of the interface of the catalyst to the liquid aqueous phase as well as the operation parameter will affect the frequency range and the size of noise in the EIS.

Characterization and Erosion Modeling of a Nozzle-Based Inflow-Control Device

In the petroleum industry, water-and-gas breakthrough in hydrocarbon reservoirs is a common issue that eventually leads to uneconomic production. To extend the economic production lifetime, inflow-control devices (ICDs) are designed to delay the water-and-gas breakthrough. Because the lifetime of a hydrocarbon reservoir commonly exceeds 20 years and it is a harsh environment, the reliability of the ICDs is vital.
Chemical and Electrochemical Properties of La$_{0.58}$Sr$_{0.4}$Fe$_{0.8}$Co$_{0.2}$O$_{3-\delta}$ (LSCF) Thin Films upon Oxygen Reduction and Evolution Reactions

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

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

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**Chemical Editing of Macro cyclic Natural Products and Kinetic Profiling Reveal Slow, Tight-Binding Histone Deacetylase Inhibitors with Picomolar Affinities**

Histone deacetylases (HDACs) are validated targets for treatment of certain cancer types and play numerous regulatory roles in biology, ranging from epigenetics to metabolism. Small molecules are highly important as tool compounds for probing these mechanisms as well as for the development of new medicines. Therefore, detailed mechanistic information and precise characterization of the chemical probes used to investigate the effects of HDAC enzymes are vital. We interrogated Nature’s arsenal of macrocyclic nonribosomal peptide HDAC inhibitors by chemical synthesis and evaluation of more than 30 natural products and analogues. This furnished surprising trends in binding affinities for the various macrocycles, which were then exploited for the design of highly potent class I and IIb HDAC inhibitors. Furthermore, thorough kinetic investigation revealed unexpected inhibitory mechanisms of important tool compounds as well as the approved drug Istodax (romidepsin). This work provides novel inhibitors with varying potencies, selectivity profiles, and mechanisms of inhibition and, importantly, affords insight into known tool compounds that will improve the interpretation of their effects in biology and medicine.
Chemical Production of Graphene Catalysts for Electrochemical Energy Conversion

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

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Chemical Synthesis and Electrochemical Characterization of Nanoporous Gold films
Nanoporous gold (NPG) is conventionally made via dealloying methods. We present an alternative method for bottom-up chemical synthesis of nanoporous gold film (cNPGF), with properties resembling those of dealloyed NPG. The developed procedure is simple and only benign chemicals are used. Chloroauric acid is reduced to nanoparticles (NPs) by 2-(N-morpholino)ethanesulfonate, acting also as a protecting agent for the NPs and as a pH buffer, while potassium chloride is used to control ionic strength. The film formation is controlled by parameters such as temperature, ionic strength and protonation of the buffer. Therefore, it is possible to influence the trapping of nanoparticles at the air-liquid interface, yielding porous thin film structures, Figure 1A. The produced cNPGFs have been investigated by atomic force microscopy (AFM), transmission electron microscopy (TEM) and cyclic voltammetry (CV). The micro- and nanostructure of cNPGFs are shown in Figure 1B and 1C. The film coverage areas that we can achieve are up to 20 cm2, with an average thickness of 500 ± 200 nm. It is also found that in-house synthesized cNPGFs are active electrocatalysts for CO2 reduction and CO oxidation.

General information
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Organisations: Department of Chemistry, NanoChemistry, Organic Chemistry, Technical University of Denmark
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Chemical Synthesis of Oligosaccharides related to the Cell Walls of Plants and Algae

Plant cell walls are composed of an intricate network of polysaccharides and proteins that varies during the developmental stages of the cell. This makes it very challenging to address the functions of individual wall components in cells, especially for highly complex glycans. Fortunately, structurally defined oligosaccharides can be used as models for the glycans, to study processes such as cell wall biosynthesis, polysaccharide deposition, protein-carbohydrate interactions, and cell-cell adhesion. Synthetic chemists have focused on preparing such model compounds, as they can be produced in good quantities and with high purity. This review contains an overview of those plant and algal polysaccharides, which have been elucidated to date. The majority of the content is devoted to detailed summaries of the chemical syntheses of oligosaccharide fragments of cellulose, hemicellulose, pectin, and arabinogalactans, as well as glycans unique to algae. Representative synthetic routes within each class are discussed in detail and the progress in carbohydrate chemistry over recent decades is highlighted.

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Chemoenzymatic synthesis of fluorogenic phospholipids and evaluation in assays of phospholipases A, C and D

Phospholipases are ubiquitous in nature and the target of significant research aiming at both their physiological roles and technical applications in e.g. the food industry. In the search for sensitive and selective phospholipase assays, we have focused on synthetic FRET (Forster resonance energy transfer) substrates. This has led to the development of a facile, easily scalable and low cost synthesis of fluorogenic phospholipids featuring the dansylidabcyl fluorophore/quencher-pair on the fatty acid co-position and on the phosphatidylethanolamine head group, respectively. Hence, the two substrates lyso-(dansyl-FA)-GPE-dabcyl (6) and (dansyl-FA)₂-GPE-dabcyl (7) were synthesized by a chemoenzymatic strategy, in which preparation of (6) further included a novel selective enzymatic esterification step. As proof of concept, activity of a handful of phospholipases, one from each of the PLA1, PLA2, PLC and PLO classes, were assayed using substrates (6) and (7), and the kinetic parameter $k_{cat}/K_M$ was determined. The PLA1 (Lecitase Ultra™) was found to be highly active on both substrates, whereas the PLO (from white cabbage) had no activity, presumably due to steric effects associated with the dabcyl-functionalization of the head group. It was further substantiated that the substrates are specific towards phospholipase activity as the tested lipase (Lipolase™) showed close to zero activity.

General information

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Authors: Piel, M. S. (Ekstern), Peters, G. H. (Intern), Brask, J. (Intern)
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Chemoselective Synthesis of Dithioacetals from Bio-aldehydes with Zeolites under Ambient and Solvent-free Conditions

Dithioacetals are an important class of versatile compounds extensively applied in pharmaceuticals, separations, electrochemistry, and organic synthesis, but few heterogeneous catalytic systems are reported to be generally applicable for their synthesis from a wide range of substrates. A series of commercial and modified zeolites are excellent catalysts for thioacetalization of different thiols with carbonyl compounds, including biomass-derived aldehydes, at room temperature under solvent-free conditions. A near quantitative yield of dithioacetal was obtained over H-beta(19) at room temperature with a low catalyst to substrate ratio of 1:19, and a method to follow the reaction progress by ex situ UV/Vis absorption analysis was demonstrated. Recycling experiments with H-beta(19) in five consecutive runs resulted in slight loss of activity, but the original activity could be fully restored after calcination at 550 degrees C. The results and physicochemical properties of the zeolites revealed that relatively large pores and moderate acidity with an appropriate distribution of Bronsted/Lewis acid sites contributed to the pronounced performance in the dithioacetal formation.
Comment on "Density functional theory is straying from the path toward the exact functional"

Medvedev et al (Reports, 6 January 2017, p. 49) argue that recent density functionals stray from the path toward exactness. This conclusion rests on very compact 1s^2 and 1s^22s^2 systems favored by the Hartree-Fock picture. Comparison to actual energies for the same systems indicates that the "straying" is not chemically relevant and is at best specific to the studied dense systems.

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Comparison of GERG-2008 and simpler EoS models in calculation of phase equilibrium and physical properties of natural gas related systems

Accurate description of thermodynamic properties of natural gas systems is of great significance in the oil and gas industry. For this application, non-cubic equations of state (EoSs) are advantageous due to their better density and compressibility description. Among the non-cubic models, GERG-2008 is a new wide-range EoS for natural gases and other mixtures of 21 natural gas components. It is considered as a standard reference equation suitable for natural gas applications where highly accurate thermodynamic properties are required. Soave's modification of Benedict-Webb-Rubin (Soave-BWR) EoS is another model that despite its empirical nature, provides accurate density description even around the critical point. It is much simpler than GERG-2008 and easier to handle and generalize to reservoir oil fluids. This study presents a comprehensive comparison between GERG-2008 and other cubic (SRK and PR) and noncubic EoSs (Soave-BWR and PC-SAFT) with a focus on Soave-BWR in description of pure components density and compressibility in a wide temperature and pressure range, calculation of binary Vapor-Liquid-Equilibria (VLE) and density, prediction of multicomponent phase envelopes and gas compressibility factor. In addition, the performance of GERG-2008 is compared with that of cubic and non-cubic models in calculation of thermal properties such as heat capacity and Joule-Thomson coefficient for pure components and multicomponent mixtures over a wide pressure and temperature range. The results are compared with available experimental data in the literature and special emphasis has been given to the reverse Joule-Thomson effects at high pressure high temperature (HPHT) conditions. © 2016 Elsevier B.V. All rights reserved.
THz absorption spectra have been recorded for the weakly bound molecular complexes of H2O with C2H4 and C2H2 embedded in cryogenic neon matrices at 2.8 K. The observation and assignment of a large-amplitude acceptor OH librational mode of the C2H2—H2O complex at 145.5 cm^{-1} confirms an intermolecular CH⋯O hydrogen-bonded configuration of C2v symmetry with the H2O subunit acting as the hydrogen bond acceptor. The observation and assignment of two large-amplitude donor OH librational modes of the C2H4—H2O complex at 255.0 and 187.5 cm^{-1}, respectively, confirms an intermolecular OH⋯π hydrogen-bonded configuration with the H2O subunit acting as the hydrogen bond donor to the π-cloud of C2H4. A (semi)-empirical value for the change of vibrational zero-point energy of 4.0–4.1 kJ mol^{-1} is proposed and the combination with quantum chemical calculations at the CCSD(T)-F12b/aug-cc-pVQZ level provides a reliable estimate of 7.1 ± 0.3 kJ mol^{-1} for the dissociation energy D_0 of the C2H4—H2O complex. In addition, tentative assignments for the two strongly infrared active OH librational modes of the ternary C4H4—HOH—C2H4 complex having H2O as a doubly OH⋯π hydrogen bond donor are proposed at 213.6 and 222.3 cm^{-1}. The present findings demonstrate that the relative stability of the weak hydrogen bond motifs is not entirely rooted in differences of electronic energy but also to a large extent by differences in the vibrational zero-point energy contributions arising from the class of large-amplitude intermolecular modes.
Competition of van der Waals and chemical forces on gold–sulfur surfaces and nanoparticles

Chemists generally believe that covalent and ionic bonds form much stronger links between atoms than the van der Waals force does. However, this is not always so. We present cases in which van der Waals dispersive forces introduce new competitive bonding possibilities rather than just modulating traditional bonding scenarios. Although the new possibilities could arise from any soft–soft chemical interaction, we focus on bonding between gold atoms and alkyl or arylsulfur ligands, RS. Consideration of all the interactions at play in sulfur-protected gold surfaces and gold nanoparticles is necessary to understand their structural, chemical and spectroscopic properties. In turn, such knowledge opens pathways to new chemical entities and innovative nanotechnological devices. Such experimentation is complemented by modern theory, and presented here is a broad overview of computational methods appropriate to fields ranging from gas-phase chemistry to device physics and biochemistry.

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Complete elimination of nonlinear light-matter interactions with broadband ultrafast laser pulses

The absorption of a single photon that excites a quantum system from a low to a high energy level is an elementary process of light-matter interaction, and a route towards realizing pure single-photon absorption has both fundamental and practical implications in quantum technology. Due to nonlinear optical effects, however, the probability of pure single-photon absorption is usually very low, which is particularly pertinent in the case of strong ultrafast laser pulses with broad bandwidth. Here we demonstrate theoretically a counterintuitive coherent single-photon absorption scheme by eliminating nonlinear interactions of ultrafast laser pulses with quantum systems. That is, a completely linear response of the system with respect to the spectral energy density of the incident light at the transition frequency can be obtained for all transition probabilities between 0 and 100% in multilevel quantum systems. To that end, a multiobjective optimization algorithm is developed to find an optimal spectral phase of an ultrafast laser pulse, which is capable of eliminating all possible nonlinear optical responses while maximizing the probability of single-photon absorption between quantum states. This
work not only deepens our understanding of light-matter interactions, but also offers a way to study photophysical and photochemical processes in the “absence” of nonlinear optical effects.
Convenient and Sustainable Hydrogen Storage using Liquid Organic Hydrogen Carrier (LOHC) Technologies

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Convenient one-step synthesis of 5-carboxy-seminaphthofluoresceins
The one-step synthesis and characterization of a series of regioisomerically pure 5-carboxy-seminaphthofluoresceins (5-carboxy-SNAFLs) is reported. The optical properties were determined in aqueous buffer at around biological pH, and highly pH sensitive, large Stokes-shift fluorophores with emission in the deep-red to near-infrared region were identified

General information
State: Published
Organisations: Department of Chemistry, Center for Nanomedicine and Theranostics, X-ray Crystallography, Department of Micro- and Nanotechnology, Colloids and Biological Interfaces, Organic Chemistry, Lund University
Authors: Hammershøj, P. (Intern), Thyhaug, E. (Ekstern), Harris, P. (Intern), Ek, P. K. (Intern), Andresen, T. L. (Intern), Clausen, M. H. (Intern)
Pages: 1611-1615
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Tetrahedron Letters
Volume: 58
Issue number: 16
ISSN (Print): 0040-4039
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.13 SJR 0.754 SNIP 0.635
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.757 SNIP 0.747 CiteScore 2.3
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.794 SNIP 0.796 CiteScore 2.41
Convergent strategy for the synthesis of S-linked oligoxylans

Arabinoxylans (AX) are a major class of hemicellulose and an important polysaccharide component of lignocellulosic biomass. To utilize the glycan polymer effectively, it is desirable to learn more about the enzymatic hydrolysis of AXs. Well-defined glycans can help to elucidate these processes. Here, we report the efficient synthesis of a mixed O- and S-linked tetraxylan. This thio-oligosaccharide has been developed as a putative inhibitor of arabinoxylan degrading enzymes used for the saccharification of biomass. Two common approaches for the synthesis of thio-oligosaccharides, either involving 1-thioglycoside donors or thioacceptors, are presented and compared regarding byproduct formation and yields. Both methods have shown to be useful for the synthesis of thiolinkages in oligoxylans assembly. However, the success of the reaction is highly dependent on the “match” between donors and acceptors.

Association of photoswitch within curcubit[7]- and [8]uril tunes the kinetics of the thermal isomerization from VHF-to-DHA in the photoswitch. The sun setting through the rolling wave symbolizes the aqueous medium in which the photoswitching processes take place. More information can be found in the Full Paper by M. B. Nielsen, S. R. Beeren, M. Pittelkow et al. on page 17010.

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry, University of Copenhagen
Authors: Petersen, M. Á. (Ekstern), Rasmussen, B. (Ekstern), Andersen, N. N. (Ekstern), Sauer, S. P. A. (Ekstern), Nielsen, M. B. (Ekstern), Beeren, S. R. (Intern), Pittelkow, M. (Ekstern)
Pages: 16916-16916
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Chemistry: A European Journal
Volume: 23
Issue number: 67
ISSN (Print): 0947-6539
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 5.03 SJR 2.247 SNIP 1.046
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 2.416 SNIP 1.184 CiteScore 4.99
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.487 SNIP 1.219 CiteScore 5.51
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.604 SNIP 1.239 CiteScore 5.68
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 2.884 SNIP 1.294 CiteScore 5.55
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 2.726 SNIP 1.336 CiteScore 5.46
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 2.527 SNIP 1.292
dDNP as an emerging real time analytical method for catalytic reactions

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry, Department of Electrical Engineering, Center for Hyperpolarization in Magnetic Resonance
Number of pages: 1
Publication date: 2017
Event: Abstract from EUROMAR 2017, Warsaw, Poland.
Main Research Area: Technical/natural sciences
Electronic versions:
Abstract_PANBO_Euromar_17.pdf

Relations
Activities:
dDNP as an emergent real time analytical method for catalytic reactions
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2017

Deactivation of SCR catalysts by potassium: A study of potential alkali barrier materials
The use of coatings in order to protect vanadia based SCR catalysts against potassium poisoning has been studied by lab- and pilot-scale experiments. Three-layer pellets, consisting of a layer of a potential coating material situated between layers of fresh and potassium poisoned SCR catalyst, were used to test the ability of the barrier layer to block the diffusion of potassium across the pellet. Of MgO, sepiolite and Hollandite manganese oxide, MgO was the most effective potassium barrier, and no potassium was detected in the MgO layer upon exposure to SCR conditions for 7 days. Two monoliths
have been exposed to KCl aerosols at 350 °C in a pilot-scale setup for about 1000 hours. A 3 wt.% V₂O₅-7 wt.% WO₃ /TiO₂ reference catalyst deactivated with an average rate of 0.91 %/day, and SEM-EDS analysis showed complete potassium penetration of the catalyst wall. A similar monolith coated with 8.06 wt.% MgO deactivated with a rate of only 0.24 %/day, relative to the fresh activity of the uncoated reference. The initial observed activity of the coated catalyst was, however, only 58 % of that of the reference, likely due to increased transport limitations and loss of active material during the coating process. Potassium had to some extent penetrated the MgO coat, and SEM analysis revealed it to be rather thick and fragile. Despite these observations, the coating did protect the SCR catalyst against potassium poisoning to some degree, leaving promise of further optimization.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry, Freiberg University of Mining and Technology, Haldor Topsoe AS
Authors: Olsen, B. K. (Intern), Kügler, F. (Ekstern), Castellino, F. (Ekstern), Schill, L. (Intern), Jensen, A. D. (Intern)
Pages: 56-64
Publication date: 2017
Main Research Area: Technical/natural sciences

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.

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry
Authors: Mielby, J. J. (Intern), Kunov-Kruse, A. J. (Intern), Kegnæs, S. (Intern)
Pages: 149-156
Publication date: 2017
Main Research Area: Technical/natural sciences
Publication information
Journal: Journal of Catalysis
Volume: 345
ISSN (Print): 0021-9517
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 7.27 SJR 2.441 SNIP 2.154
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 2.703 SNIP 2.198 CiteScore 7.23
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.685 SNIP 2.25 CiteScore 6.92
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.56 SNIP 2.108 CiteScore 6.42
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 3.005 SNIP 2.277 CiteScore 6.17
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 3.11 SNIP 2.207 CiteScore 6.23
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 3.376 SNIP 2.213
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.951 SNIP 2.158
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 3.115 SNIP 2.184
Web of Science (2008): Indexed yes
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 3.129 SNIP 2.023
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 2.986 SNIP 2.16
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 2.64 SNIP 1.964
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 2.147 SNIP 1.87
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 2.49 SNIP 1.803
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 2.943 SNIP 1.931
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 2.85 SNIP 2.22
Density and Compressibility of Multicomponent n-Alkane Mixtures up to 463 K and 140 MPa

Density measurements of two ternary alkane mixtures (methane/n-butane/n-decane and methane/n-butane/n-dodecane) and two multicomponent mixtures composed of methane/n-butane/n-octane/n-dodecane/n-hexadecane/n-eicosane were performed in the temperature range from (278.15 to 463.15) K and pressures up to 140 MPa. The isothermal compressibility values of these mixtures were obtained by differentiation from a Tait-type fitting of experimental densities as a function of temperature and pressure. Excess volume of the studied mixtures was also determined. Four different equations of state, that is, Soave–Redlich–Kwong (SRK), Peng–Robinson (PR), Perturbed Chain Statistical Associating Fluid Theory (PC-SAFT), and Soave-Benedit-Webb-Rubin (Soave-BWR) were used for predicting the experimental density values as well as the excess volumes.

General information
State: Accepted/In press
Organisations: Department of Chemistry, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, Technical University of Denmark
Authors: Regueira, T. (Intern), Glykioti, M. (Ekstern), Stenby, E. H. (Intern), Yan, W. (Intern)
Number of pages: 9
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Chemical and Engineering Data
ISSN (Print): 0021-9568
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.29 SJR 0.88 SNIP 1.097
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.868 SNIP 0.966 CiteScore 1.96
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.021 SNIP 1.208 CiteScore 2.22
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.135 SNIP 1.199 CiteScore 2.17
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.141 SNIP 1.103 CiteScore 2.01
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.862 SNIP 0.988 CiteScore 1.8
ISI indexed (2011): ISI indexed yes
Design of sintering-stable heterogeneous catalysts

One of the major issues in the use of metal nanoparticles in heterogeneous catalysis is sintering. Sintering occurs at elevated temperatures because of increased mobility of nanoparticles, leading to their agglomeration and, as a consequence, to the deactivation of the catalyst. It is an emerging problem especially for the noble metals-based catalysis. These metals being expensive and scarce, it is worth developing catalyst systems which preserve their activity over time. Encapsulation of nanoparticles inside zeolites is one of the ways to prevent sintering. Entrapment of nanoparticles inside the crystalline framework of a zeolite creates a steric hindrance against agglomeration into larger clusters. In the present study, experimental protocols for encapsulation of metal nanoparticles inside zeolites were developed. Two different methodologies were proposed to encapsulate gold, palladium and platinum nanoparticles inside silicalite-1 - the pressure assisted impregnation and reduction method (PAIR), and in situ incorporation method. PAIR is based on modified incipient wetness impregnation technique in which the impregnation of a zeolite with a solution of metal precursor and its reduction are performed under elevated pressure. In situ incorporation is a one-pot procedure based on simultaneous growth of a zeolite and entrapment of metal precursor in a form of ethylenediamine complex inside the forming crystalline network, leading to encapsulated metal nanoparticles after reduction in hydrogen. The PAIR procedure was used to successfully synthesize gold nanoparticles, 2-3 nm in size inside silicalite-1 and ZSM-5. Silicalite-1 with 2 nm palladium nanoparticles uniformly distributed on the external surface of the crystal was synthesized as well using the PAIR method. The in situ incorporation method was used to produce single metal palladium and platinum nanoparticles, 2-3 nm in size, and bi-metallic palladium/platinum nanoparticles inside silicalite-1. Materials were primarily characterized using XRD, nitrogen physisorption, TEM, and XRF techniques. STEM and XPS were also used in selected cases. Synthesized catalysts were able to decompose formic acid with ~ 85% selectivity towards hydrogen at temperatures around 100 °C. Palladium/silicalite-1 catalysts were shown to be very active in Suzuki cross-coupling reaction of bromobenzene and 4-methoxyphenylboronic acid in methanol at 70 °C reaching yields of ~ 85% after 45 min. Oxidation of allyl alcohol to its methyl esters at ambient conditions showed a very low activity of gold/silicalite-1 catalyst due to limited diffusion and possible adsorption of products inside the pores of zeolite. It was shown that the PAIR method and in situ incorporation method are feasible and easy protocols for synthesis of metal nanoparticles encapsulated inside a zeolite matrix. Small size, stability towards sintering and high activity of nanoparticles obtained using the PAIR method and in situ incorporation method makes these two protocols promising for further research.
Detecting Elusive Intermediates in Carbohydrate Conversion: A Dynamic Ensemble of Acyclic Glucose-Catalyst Complexes

The role of acyclic carbohydrates in pathways towards value-added chemicals has remained poorly characterized due to the low population of acyclic forms, and due to their instability under reaction conditions. We conduct steady-state and pre-steady state measurements by direct reaction progress monitoring with sensitivity-optimized NMR spectroscopy in the molybdate-catalyzed epimerization of glucose to mannose. We detect an exchanging pool of at least five acyclic glucose-catalyst complexes under near-optimum reaction conditions. In the presence of catalyst, the acyclic glucose population increases within few seconds prior to reaching a steady state. Exchange between the acyclic intermediates increases at conditions that favor epimerization. Species accounting for less than 0.05% of total glucose can be monitored with sub-second time resolution to allow kinetic analysis of intermediate formation and catalytic conversion. Epimerization occurs 2-3 orders of magnitude-fold faster than the binding of acyclic glucose to the catalyst at near-optimum reaction conditions. The current study brings insight into the nature of acyclic intermediate-catalyst complexes of very low population and into experimental strategies for characterizing very minor intermediates in carbohydrate conversion to value-added compounds.

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry, Center for Hyperpolarization in Magnetic Resonance, Department of Electrical Engineering, Center for Magnetic Resonance
Authors: Meier, S. (Intern), Karlsson, M. (Intern), Jensen, P. R. (Intern)
Pages: 5571-5577
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: ACS Sustainable Chemistry & Engineering
Volume: 5
Issue number: 6
ISSN (Print): 2168-0485
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 5.92 SJR 1.523 SNIP 1.408
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.381 SNIP 1.338 CiteScore 5.39
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.195 SNIP 1.207 CiteScore 4.3
Web of Science (2014): Indexed yes
Determination of Zinc Sulfide Solubility to High Temperatures

A new experimental set-up and methodology for the measurement of ZnS solubility in aqueous solutions at 40, 60 and 80 °C (atmospheric pressure) is presented. The methodology implemented includes the preparation of the samples in a reduced oxygen atmosphere, particle size analysis of ZnS, quality control of the analytical technique and evaluation of equilibration time. ZnS solubility analyses were run for prolonged times (up to 11 days) to ensure that equilibrium conditions were met. The equilibration time was explored at three temperatures (40, 60 and 80 °C) observing small variations in the time required to reach the solid–liquid equilibrium at each temperature. Equilibrium was reached within 72 h. The concentration of zinc and of total sulfur were determined using Inductively Coupled Plasma Optical Emission Spectroscopy (ICP-OES). The experimental solubility data show an exponential dependency of the solubility with respect to temperature. An increase of 40 °C results in an increase of roughly 12 times for the solubility of ZnS.
Development of a UV-Cleavable Protecting Group for Hydroxylamines, Synthesis of a Structurally Wide Variety of Hydroxamic Acids, and Identification of Histone Deacetylase Inhibitors

Photo-cleavable protecting groups are highly applicable for the synthesis of structural complex and sensitive compounds, including biological important molecules. Herein, we present the development of a novel O-hydroxylamine photo-cleavable protecting group, based on the methyl-6-nitroveratryl moiety. We demonstrate the application of the protected hydroxylamine derivative for the synthesis of N-alkylated hydroxamic acids. We have shown that the construct is stable toward a diverse set of reaction conditions, as well as orthogonal with conventional protection groups. The O-protected hydroxylamine derivative was applied to synthesize a small collection of N-alkylated hydroxamic acids as inhibitors of the histone deacetylase enzymes, an important class of enzymes for the treatment of a range of diseases, most importantly cancer. During my external stay at Nanyang Technological University, Singapore, I worked on a project with the aim of synthesizing compounds that target the quorum sensing network in Pseudomonas aeruginosa, important for the treatment of bacterial infections. The structure was based on a recent found hit compound, by our collaborators in Singapore, showing high activity.

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry
Authors: Mortensen, K. T. (Intern), Qvortrup, K. (Intern), Nielsen, T. E. (Intern)
Number of pages: 271
Publication date: 2017

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

Relations
Projects:
Development of a UV-Cleavable Protecting Group for Hydroxylamines, Synthesis of a Structurally Wide Variety of Hydroxamic Acids, and Identification of Histone Deacetylase Inhibitors
Publication: Research › Ph.D. thesis – Annual report year: 2017

Diastereoselective Synthesis of Novel Heterocyclic Scaffolds through Tandem Petasis 3-Component/Intramolecular Diels-Alder and ROM-RCM Reactions
A high-yielding, stereoselective and extraordinarily complexity generating Petasis 3-component/intramolecular Diels-Alder reaction has been developed. In combination with ROM-RCM, rapid access to complex sp²-rich heterocyclic
scaffolds amenable to subsequent functionalization and library synthesis is provided.

**General information**
State: Published
Organisations: Department of Chemistry, Organic Chemistry
Authors: Ishøy, M. (Intern), Petersen, R. (Intern), Petersen, M. Å. (Intern), Wu, P. (Intern), Clausen, M. H. (Intern), Nielsen, T. E. (Intern)
Number of pages: 4
Pages: 9410-9413
Publication date: 2017
Main Research Area: Technical/natural sciences

**Publication information**
Journal: Chemical Communications
Volume: 53
Issue number: 68
ISSN (Print): 1359-7345
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
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
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
Scopus rating (2006): SJR 2.366 SNIP 1.183
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 2.129 SNIP 1.15
Dispersive Molecular Imprinting of Proteins for the Production of Plastic Antibodies

General information
State: Published
Organisations: Department of Micro- and Nanotechnology, NanoChemistry
Authors: Ashley, J. (Intern), Feng, X. (Intern), Halder, A. (Intern), Zhou, T. (Intern), Sun, Y. (Intern)
Number of pages: 1
Publication date: 2017

Host publication information
Title of host publication: Book of Abstracts, Sustain 2017
Publisher: Technical University of Denmark (DTU)
Article number: H-2
Main Research Area: Technical/natural sciences
Conference: Sustain 2017, Kgs. Lyngby, Denmark, 06/12/2017 - 06/12/2017
Electronic versions:
SustainAbstracts2017c.compressed_84.pdf
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2017

Disulfide Bond-Containing Ajoene Analogues As Novel Quorum Sensing Inhibitors of Pseudomonas aeruginosa
Since its discovery 22 years ago, the bacterial cell-to-cell communication system, termed quorum sensing (QS), has shown potential as antipathogenic target. Previous studies reported that ajoene from garlic inhibits QS in opportunistic human pathogen Pseudomonas aeruginosa. In this study, screening of an in-house compound library revealed two sulfur-containing compounds which possess structural resemblance with ajoene and inhibit QS in bioReporter assay. Following a quantitative structure-activity relationship (SAR) study, 25 disulfide bond-containing analogues were synthesized and tested for QS inhibition activities. SAR study indicated that the allyl group could be replaced with other substituents, with the most active being benzothiazole derivative (IC50 = 0.56 μM). The compounds were able to reduce QS-regulated virulence factors (elastase, rhamnolipid, and pyocyanin) and successfully inhibit P. aeruginosa infection in murine model of implant-associated infection. Altogether, the QS inhibition activity of the synthesized compounds is encouraging for further exploration of novel analogues in antimicrobial drug development.

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry, Nanyang Technological University, University of Copenhagen
Authors: Fong, J. (Ekstern), Yuan, M. (Ekstern), Jakobsen, T. H. (Ekstern), Mortensen, K. T. (Intern), Delos Santos, M. M. S. (Ekstern), Chua, S. L. (Ekstern), Yang, L. (Ekstern), Tan, C. H. (Ekstern), Nielsen, T. E. (Ekstern), Givskov, M. (Ekstern)
Number of pages: 13
Pages: 215–227
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Medicinal Chemistry
Volume: 60
DNP NMR of carbohydrate converting enzymes

Dissolution dynamic nuclear polarization (DNP) NMR can be used to increase the sensitivity of $^{13}$C NMR signal by up to four orders of magnitude. This allows for real time monitoring of reactions and observation of intermediates. The biggest drawback of the method is the loss of polarization with $T_1$ relaxation, but even with this limitation, it is possible to obtain
detailed reaction parameters in less than one minute. The enzyme investigated was β-galactosidase from E. coli (E.C. 3.2.1.23). It is well described and the mechanism is generally accepted to be a double displacement with a covalently bound intermediate, however, this evidence is based on mutant of X-ray crystallography and simulations. As the natural substrate lactose does not have any quaternary carbon with long T1, the unnatural substrate o-nitrophenyl β-D-galactopyranoside was used (figure 1) as the quaternary positions have T1 relaxations of ca. 15 s instead of <2 s. The DNP NMR monitoring of the hydrolysis of this substrate can be seen in figure 2, and another use of this substrate is for optimizing the conditions for a labelled substrate (figure 1), which would further increase the signal and allow monitoring of the carbohydrate instead of the aglycon. This is, however, not commercially available and had to be synthesized from doubly labelled galactose.

**General information**
State: Published
Organisations: Department of Chemistry, Department of Electrical Engineering, Center for Hyperpolarization in Magnetic Resonance, Organic Chemistry
Authors: Kjeldsen, C. (Intern), Ardenkjær-Larsen, J. H. (Intern), Duus, J. Ø. (Intern)
Publication date: 2017
Event: Abstract from 19th European Carbohydrate Symposium, Barcelona, Spain.
Main Research Area: Technical/natural sciences
Electronic versions:
LIBRO_COMPLETO_EUROCARB6.pdf
Publication: Research - peer-review » Conference abstract for conference – Annual report year: 2017

**Drastic difference between hole and electron injection through the gradient shell of CdSeZnS quantum dots**
Ultrafast fluorescence spectroscopy was used to investigate the hole injection in CdSeZnS gradient core-shell quantum dot (CSQD) sensitized p-type NiO photocathodes. A series of CSQDs with a wide range of shell thicknesses was studied. Complementary photoelectrochemical cell measurements were carried out to confirm that the hole injection from the active core through the gradient shell to NiO takes place. The hole injection from the valence band of the QDs to NiO depends much less on the shell thickness when compared to the corresponding electron injection to n-type semiconductor (ZnO). We simulate the charge carrier tunneling through the potential barrier due to the gradient shell by numerically solving the Schrödinger equation. The details of the band alignment determining the potential barrier are obtained from X-ray spectroscopy measurements. The observed drastic differences between the hole and electron injection are consistent with a model where the hole effective mass decreases, while the gradient shell thickness increases.

**General information**
State: Published
Organisations: NanoChemistry, Department of Chemistry, Organic Chemistry, Lund University, University of Copenhagen , Academy of Sciences of the Czech Republic, Uppsala University, Deutsches Elektronensynchrotron DESY
Pages: 12503-12508
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**Publication information**
Journal: Nanoscale
Volume: 9
Issue number: 34
ISSN (Print): 2040-3364
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BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 7.46 SJR 2.769 SNIP 1.459
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 2.842 SNIP 1.588 CiteScore 7.97
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.651 SNIP 1.676 CiteScore 7.64
Effect of carbon on interstitial ordering and magnetic properties of ε-Fe2(N,C)1-z

Hexagonal ε-iron nitride and ε-iron carbonitride phases are formed on nitriding and nitrocarburizing of iron and steel surfaces and can exist in broad compositional ranges. Long-range nitrogen ordering and magnetic properties for ε-iron nitrides and their dependence on composition have been the focus of several studies. So far, limited attention has been paid to the carbonitrides. In the current work, the effects of substitution of nitrogen by carbon on the interstitial ordering and magnetic properties in Fe2(C,N)1-z are explored using neutron diffraction, Mössbauer spectroscopy and vibrating sample magnetometry. Neutron diffraction patterns showed 001 and 301 superstructure reflections, confirming a previously proposed structural model in space group P31m (compared to P6322 for the pure nitrides). On partial substitution of nitrogen by carbon in ε-iron nitride the Curie temperature, the saturation magnetization and the hyperfine fields of the iron atoms are increased, while isomer shifts are decreased. The effects on the a and c lattice parameters indicate a change in interstitial ordering, which is related to more favorable interactions between a nitrogen and carbon atom than among nitrogen atoms. This interaction leads to additional interstitial (short-range) ordering and a decrease in the c lattice parameter, while the a lattice parameter is largely unaffected.

General information
State: Published
Organisations: Department of Mechanical Engineering, Materials and Surface Engineering, Department of Physics, Neutrons and X-rays for Materials Physics, Department of Chemistry, X-ray Crystallography, Department of Micro- and Nanotechnology, Magnetic Systems, Academy of Sciences of the Czech Republic
Authors: Brink, B. (Intern), Ståhl, K. (Intern), Christiansen, T. L. (Intern), Frandsen, C. (Intern), Hansen, M. F. (Intern), Beran, P. (Ekstern), Somers, M. A. J. (Intern)
Pages: 282-291
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Main Research Area: Technical/natural sciences

Publication information
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
Effect of Water Clustering on the Activity of Candida antarctica Lipase B in Organic Medium

The effect of initial water activity of MTBE (methyl tert-butyl ether) medium on CALB (Candida antarctica lipase B) catalyzed esterification reaction is investigated using experimental methods and classical molecular dynamics (MD)
simulations. The experimental kinetic studies show that the initial reaction rate of CALB-catalyzed esterification reaction between butyric acid and ethanol decreases with increasing initial water activity of the medium. The highest rate of esterification is observed at the lowest water activity studied. MD simulations were performed to gain a molecular insight on the effect of initial water activity on the rate of CALB-catalyzed reaction. Our results show that hydration has an insignificant effect on the structure and flexibility of CALB. Rather, it appears that water molecules bind to certain regions ("hot spots") on the CALB surface and form clusters. The size of the water clusters at these hot spot regions gradually increase and expand with increasing water activity. Consequently, the surface area of CALB covered by the water molecules also increases. Specifically, our results indicate that a particular water cluster located close to the active site partially cover the binding pocket of substrate at high water activity. As a consequence, the effective concentration of substrate at the catalytic site decreases. Therefore, the reaction rate slows down with increasing water activity, which correlates well with the observed decrease in the experimentally determined initial reaction rate.

**General information**
State: Published
Organisations: Department of Chemistry, Department of Chemical and Biochemical Engineering, PROSYS - Process and Systems Engineering Centre, KT Consortium
Authors: Banik, S. D. (Intern), Nordblad, M. (Intern), Woodley, J. M. (Intern), Peters, G. H. (Intern)
Publication date: 2017
Main Research Area: Technical/natural sciences

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Journal: Catalysts
Volume: 7
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Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.44 SJR 0.928 SNIP 1.217
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.076 SNIP 1.246 CiteScore 3.45
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.683 SNIP 1.074 CiteScore 2.17
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.521 SNIP 0.582
Scopus rating (2012): SJR 0.471 SNIP 0.358
Original language: English
Candida antarctica Lipase B, Computational Study, Kinetics Study, Water activity
Electronic versions:
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**Bibliographical note**
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**Electrical Double-Layer and Ion Bridging Forces between Symmetric and Asymmetric Charged Surfaces in the Presence of Mono- and Divalent Ions**
An atomic force microscope, employing the colloidal probe technique, was used to study the interactions between six different combinations of silane-functionalized silica surfaces in NaCl and CaCl2 solutions. The surfaces consisted of monolayers of the apolar trimethoxy(octyl)silane, the positively charged (3-aminopropyl)trimethoxysilane, and the negatively charged (3-mercaptopropyl)trimethoxysilane. The interactions between the three symmetric systems, as well as between the three asymmetric combinations of surfaces, were measured and compared to calculated electrical double-layer forces. The results demonstrated that the long-range interactions between the surfaces in all cases were dominated
by double-layer forces, while short-range interactions, including adhesion, were dominated by ion bridging forces in the cases where both interaction surfaces favored adsorption of calcium ions. The study thus also demonstrates how surface force studies in mono- and divalent salt solutions can be used as an analytical tool for probing specific functional groups on heterogeneous surfaces.

**General information**

State: Published
Organisations: Department of Chemistry, Centre for oil and gas – DTU, Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering
Authors: Liu, X. (Intern), Feilberg, K. L. (Intern), Yan, W. (Intern), Stenby, E. H. (Intern), Thormann, E. (Intern)
Number of pages: 9
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Publication date: 2017
Main Research Area: Technical/natural sciences

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Web of Science (2018): Indexed yes
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BFI (2016): BFI-level 2
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2016): CiteScore 3.99 SJR 1.55 SNIP 1.188
Web of Science (2016): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.816 SNIP 1.391 CiteScore 4.59
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.895 SNIP 1.356 CiteScore 4.55
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
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Scopus rating (2012): SJR 2.177 SNIP 1.382 CiteScore 4.37
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BFI (2011): BFI-level 2
Scopus rating (2011): SJR 2.051 SNIP 1.357 CiteScore 4.42
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 2.148 SNIP 1.4
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.156 SNIP 1.351
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 2.383 SNIP 1.34
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 2.449 SNIP 1.434
Web of Science (2007): Indexed yes
Electroactive and biocompatible functionalization of graphene for the development of biosensing platforms

Design and synthesis of low-cost, highly stable, electroactive and biocompatible material is one of the key steps for the advancement of electrochemical biosensing systems. To this end, we have explored a facile way for the successful synthesis of redox active and bioengineering of reduced graphene oxide (RGO) for the development of versatile biosensing platform. A highly branched polymer (PEI) is used for reduction and simultaneous derivation of graphene oxide (GO) to form a biocompatible polymeric matrix on RGO nanosheet. Ferrocene redox moieties are then wired onto RGO nanosheets through the polymer matrix. The as-prepared functional composite is electrochemically active and enables to accommodate enzymes stably. For proof-of-concept studies, two crucial redox enzymes for biosensors (i.e. cholesterol oxidase and glucose oxidase) are targeted. The enzyme integrated and RGO supported biosensing hybrid systems show high stability, excellent selectivity, good reproducibility and fast sensing response. As measured, the detection limit of the biosensors for glucose and cholesterol is 5 µM and 0.5 µM (S/N=3), respectively. The linear response range of the biosensor is from 0.1 to 15.5 mM for glucose and from 2.5 to 25 µM for cholesterol. Furthermore, this biosensing platform shows good anti-interference ability and reasonable stability. The nanohybrid biosensing materials can be combined with screen-printed electrodes, which are successfully used for measuring the glucose and cholesterol level of real human serum samples.

General information
State: Published
Organisations: Department of Chemistry, NanoChemistry, Organic Chemistry
Authors: Halder, A. (Intern), Zhang, M. (Intern), Chi, Q. (Intern)
Number of pages: 8
Pages: 764-771
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Main Research Area: Technical/natural sciences

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Volume: 87
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Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 7.22 SJR 2.092 SNIP 1.633
Web of Science (2016): Indexed yes
Electrocatalysis of Gold Nanostructures for Electrochemical Energy Conversion

General information

State: Published
Organisations: Department of Chemistry, NanoChemistry, Organic Chemistry, Technical University of Denmark
Authors: Engelbrekt, C. (Intern), Seselj, N. (Intern), Christiansen, M. (Ekstern), Wagner, M. (Intern), Nielsen, F. S. (Intern), Zhang, J. (Intern)
Number of pages: 1
Publication date: 2017

Cholesterol oxidase, Electroactive functionalization, Electrochemical biosensor, Glucose oxidase, Human serum sample, Reduced graphene oxide

DOIs:
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Publication: Research - peer-review › Journal article – Annual report year: 2016
Electrocatalytic oxidation of K$_4$[Fe(CN)$_6$] by metal-reducing bacterium Shewanella oneidensis MR-1

The microbial metabolic activities between metals and bacteria play a vital role on biogeochemical cycling of metal compounds. One of these activities is extracellular electron transfer (EET), in which some microbes exchange electrons with external redox minerals, electrodes, or even other microorganisms. The bacteria can either take electrons or give electrons. Shewanella oneidensis MR-1 (MR-1) is electrochemical active, it can transfer electrons from cell to extracellular electron acceptors including Fe(III) (hydro)oxides. In this study, we report that MR-1 electrocatalyze the oxidation of an inorganic redox compound K$_4$[Fe(CN)$_6$]. A pair of symmetric peak in the cyclic voltmetry (CV) of K$_4$[Fe(CN)$_6$] were found on bare glassy carbon electrode (GCE). Surprisingly, when the GCE is coated MR-1, the anodic peak almost sustained at the same level; while the cathodic peak apparently shrunk. We attribute this phenomenon to the electrocatalytic oxidation by MR-1. The discovery of the ability to oxidize [Fe(CN)6]$^{4-}$ by MR-1 broadens our horizon of the role that dissimilatory metal reduction bacteria play in the environment.

General information
State: Published
Organisations: Department of Chemistry, NanoChemistry, Metalloprotein Chemistry and Engineering, Organic Chemistry, Chinese Academy of Sciences
Authors: Zheng, Z. (Intern), Xiao, Y. (Intern), Wu, R. (Intern), Christensen, H. E. M. (Intern), Zhao, F. (Ekstern), Zhang, J. (Intern)
Number of pages: 1
Publication date: 2017

Electrochemical Catalysis of Inorganic Complex K$_4$[Fe(CN)$_6$] by Shewanellaoneidensis MR-1

The interaction between metal and bacteria is a universal and important biogeochemical process in environment. As a dissimilatory metal reduction bacterium, the electrochemically active bacterium Shewanella oneidensis MR-1 can transfer intracellular electrons to minerals. This ability is attributed to the redox proteins localized on the outer-membrane, for example, the MtrC, MtrB, MtrA and CymA$^\text{2}$. Here we investigate its electrochemical properties towards redoxinorganic redox compounds. It shows strong electrocatalysis toward electrochemical oxidation of K$_4$[Fe(CN)$_6$]. As a redox molecule, K$_4$[Fe(CN)$_6$] gives a pair of redox peaks on voltammetry on bare glassy carbon electrode (GCE), symmetric with ideal peak-peak separation of about 60 mV, indicating ofa reversible one-electron transfer process(blue curve, Figure 1). Surprisingly, the presence of S. oneidensis MR-1 on GCE results an asymmetric redox peak, with almost disappearance of the cathodic peak and strengthen of the anodic peak, which is a typical catalysis feature of electrochemical oxidation. Further experiments show that S. oneidensis MR-1 does not give such electrocatalysis toredox compounds such as Ru[(NH)$_3$]Cl$_3$ and Resorufin. Selectivity andelectrocatalysis mechanisms of S. oneidensis MR-1 are under investigation. The ability of S. oneidensis MR-1 to catalyze redoxaction of inorganic metal complex compounds will provide an insight on metal cycles in nature.

General information
State: Published
Organisations: Department of Chemistry, NanoChemistry, Metalloprotein Chemistry and Engineering, Organic Chemistry, Chinese Academy of Sciences
Authors: Zheng, Z. (Intern), Wu, R. (Intern), Xiao, Y. (Intern), Christensen, H. E. M. (Intern), Zhao, F. (Ekstern), Zhang, J. (Intern)
Publication date: 2017

Event: Abstract from Forth EuCheMS Inorganic Chemistry Conference (EICC-4), Copenhagen, Denmark.
Main Research Area: Technical/natural sciences
Electronic versions:
Electrochemical single-molecule conductivity of duplex and quadruplex DNA

Photoinduced and electrochemical charge transport in DNA (oligonucleotides, OGNs) and the notions “hopping”, superexchange, polaron, and vibrationally gated charge transport have been in focus over more than two decades. In recent years mapping of electrochemical charge transport of pure and redox marked single- and double-strand OGNs has reached the single-molecule level based i.a. on electrochemical in situ scanning tunnelling microscopy (STM) and break-junction (B-J) STM. There are much fewer such reports on “non-canonical” OGN structures such as G-quadruplexes. We discuss first single-molecule electrochemical conductivity of pure and redox marked duplex OGNs, and address next electrochemistry and electrochemical conductivity in the few reported monolayer and single-molecule G-quadruplex studies. Facile electrochemical electron transfer of iron protoporphyrin IX stacked onto three-quartet 12-guanine quadruplex (“DNAzyme”) and in situ high-resolution molecular structures are particularly noted.

General information
State: Published
Organisations: Department of Chemistry, NanoChemistry, Organic Chemistry
Authors: Zhang, L. (Intern), Zhang, J. (Intern), Ulstrup, J. (Intern)
Pages: 66-74
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Main Research Area: Technical/natural sciences

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Source: FindIt
Source-ID: 2389682674
Publication: Research - peer-review › Journal article – Annual report year: 2017

Electrochemical Study of (La0.6Sr0.4)0.99CoO3-δ Thin Film Microelectrodes
Solid Oxide Fuel/Electrolysis Cells (SOFC/SOEC, collectively termed SOC) are one of the most promising reversible energy conversion/storage technologies. Long term durability is required for such devices to become economically feasible. One approach to make SOCs more durable and at a lower cost is to decrease the operation temperature. However, lowering the operation temperature of SOCs has shown to be challenging due to the difficulty in finding suitable oxygen electrodes which have high catalytic activity for oxygen reduction and fast ionic transport. (La,Sr)CoO3-δ (LSC) is one of the promising cathode materials due to its high electronic and ionic conductivity as well as good catalytic activity for oxygen reduction at intermediate temperatures (500-700 °C). However, LSC is characterized by low chemical stability. Multiple degradation mechanisms are reported for LSC such as zirconate formation due to reactivity with YSZ (electrolyte) at operating temperature, decomposition at low pO2, SrO enrichment of and precipitation at the surface and Cr poisoning. Several studies on the electrochemical properties of oxygen electrode materials are reported in the literature. Most of the studies are performed on porous electrodes with the purpose of having a realistic scenario; however we still lack fundamental understanding of the underlying degradation mechanism. Even though porous electrode studies have provided invaluable information about the degradation of the oxygen electrode, the deconvolution of geometrical effects from the intrinsic properties of the material is very difficult. Therefore, the presented work aims to study the oxygen reduction mechanism using geometrically well-defined dense model electrodes. Gd doped CoO2 (CGO) was deposited on polished single crystals YSZ (100) and on top of the CGO layer was deposited a (La0.6Sr0.4)0.99CoO3-δ(LSC40) using pulsed laser deposition (PLD). The thin CGO film (~100 nm) was deposited to avoid any reaction between the YSZ and LSC40 (250 nm). Subsequently, using photolithography and ion beam etching the microelectrode arrays with varying diameters (from 100 µm to 5 µm) were produced. Each sample has 4 macro-electrodes which were used as counter-electrode while performing electrochemical measurements. To observe the effect of temperature on the film microstructure and chemistry one sample was heat treated for 16 hours. SEM images, AFM and ToF-SIMS reveal similar behavior for both heat treated and as-deposited films. ToF-SIMS depth profiling reveals a Sr and Co rich surface compared to the bulk of the LSC40 for both samples. The difference between the two samples are in the distribution of common impurities, such as silica. After the heat treatment, the Si signal is higher in the LSC/CGO and CGO/YSZ interfaces (See Figure 1 a-b). The electrochemical measurements were recorded in a Controlled Atmosphere High Temperature Scanning Probe Microscope (CAHT-SPM)5which can reach temperatures up to 850 °C. The impedance spectra reveal a high frequency intercept which is related to the conductivity of the electrolyte, a small arc at high/middle frequencies originating from the electrode electrolyte interface, and finally a low frequency arc which is related to the air electrode interface. The evolution of the impedance spectra with changing temperature, atmosphere, polarization and microelectrode size combined with
surface chemical analysis and imaging techniques reveals information about the underlying degradation mechanism of LSC electrodes.

**General information**

**State:** Published  
**Organisations:** Department of Energy Conversion and Storage, Department of Chemistry  
**Authors:** Kreka, K. (Intern), Hansen, K. V. (Intern), Jacobsen, T. (Intern), Norman, K. (Intern), Chatzichristodoulou, C. (Intern), Mogensen, M. B. (Intern)  
**Publication date:** 2017  
**Event:** Abstract from 232nd ECS meeting, National Harbor, Washington, DC, United States.  
**Main Research Area:** Technical/natural sciences  
**Links:**  
http://ma.ecsd.org.proxy.findit.dtu.dk/content/MA2017-02/39/1726#aff-2  
**Source:** FindIt  
**Source-ID:** 2304160853  
**Publication:** Research - peer-review › Conference abstract for conference – Annual report year: 2017

**Electronic structure and time-dependent description of rotational predissociation of LiH**

The adiabatic potential energy curves of the $^1\Sigma^+$ and $^1\Pi$ states of the LiH molecule were calculated. They correlate asymptotically to atomic states, such as $2s + 1s$, $2p + 1s$, $3s + 1s$, $3p + 1s$, $3d + 1s$, $4s + 1s$, $4p + 1s$ and $4d + 1s$. A very good agreement was found between our calculated spectroscopic parameters and the experimental ones. The dynamics of the rotational predissociation process of the $^1\Pi$ state were studied by solving the time-dependent Schrödinger equation. The classical experiment of Velasco [Can. J. Phys., 1957, 35, 1204] on dissociation in the $^1\Pi$ state is explained for the first time in detail.

**General information**

**State:** Published  
**Organisations:** Department of Chemistry, Gdansk University of Technology, State University of Applied Sciences in Elblag  
**Authors:** Jasik, P. (Ekstern), Sienkiewicz, J. E. (Ekstern), Domsta, J. (Ekstern), Henriksen, N. E. (Intern)  
**Number of pages:** 7  
**Pages:** 19777-19783  
**Publication date:** 2017  
**Main Research Area:** Technical/natural sciences

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**ISSN (Print):** 1463-9076  
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BFI (2017): BFI-level 2  
Web of Science (2017): Indexed yes  
BFI (2016): BFI-level 2  
Scopus rating (2016): CiteScore 4.06 SJR 1.678 SNIP 1.117  
Web of Science (2016): Indexed yes  
BFI (2015): BFI-level 2  
Scopus rating (2015): SJR 1.771 SNIP 1.244 CiteScore 4.45  
Web of Science (2015): Indexed yes  
BFI (2014): BFI-level 2  
Scopus rating (2014): SJR 1.772 SNIP 1.253 CiteScore 4.29  
Web of Science (2014): Indexed yes  
BFI (2013): BFI-level 2  
Scopus rating (2013): SJR 1.715 SNIP 1.216 CiteScore 4.05  
ISI indexed (2013): ISI indexed yes  
Web of Science (2013): Indexed yes  
BFI (2012): BFI-level 2  
Scopus rating (2012): SJR 1.916 SNIP 1.184 CiteScore 3.67  
ISI indexed (2012): ISI indexed yes
Electronic Structures of LNA Phosphorothioate Oligonucleotides

Important oligonucleotides in anti-sense research have been investigated in silico and experimentally. This involves quantum mechanical (QM) calculations and chromatography experiments on locked nucleic acid (LNA) phosphorothioate (PS) oligonucleotides. Iso-potential electrostatic surfaces are essential in this study and have been calculated from the wave functions derived from the QM calculations that provide binding information and other properties of these molecules. The QM calculations give details of the electronic structures in terms of e.g., energy and bonding, which make them distinguish or differentiate between the individual PS diastereoisomers determined by the position of sulfur atoms. Rules are derived from the electronic calculations of these molecules and include the effects of the phosphorothioate chirality and formation of electrostatic potential surfaces. Physical and electrochemical descriptors of the PS oligonucleotides are compared to the experiments in which chiral states on these molecules can be distinguished. The calculations demonstrate that electronic structure, electrostatic potential, and topology are highly sensitive to single PS configuration changes and can give a lead to understanding the activity of the molecules.

General information

State: Published
Organisations: Department of Chemistry, City of Hope Medical Center, Privat consultancy, Roche Innovation Center Copenhagen
Authors: Bohr, H. G. (Intern), Shim, I. (Intern), Stein, C. (Ekstern), Ørum, H. (Ekstern), Hansen, H. F. (Ekstern), Koch, T. (Ekstern)
Pages: 428-441
Electrospun Phospholipid Fibers as Micro-Encapsulation and Antioxidant Matrices

Electrospun phospholipid (asolectin) microfibers were investigated as antioxidants and encapsulation matrices for curcumin and vanillin. These phospholipid microfibers exhibited antioxidant properties which increased after the encapsulation of both curcumin and vanillin. The total antioxidant capacity (TAC) and the total phenolic content (TPC) of curcumin/phospholipid and vanillin/phospholipid microfibers remained stable over time at different temperatures (refrigerated, ambient) and pressures (vacuum, ambient). ¹H-NMR confirmed the chemical stability of both encapsulated curcumin and vanillin within phospholipid fibers. Release studies in aqueous media revealed that the phenolic bioactives were released mainly due to swelling of the phospholipid fiber matrix over time. The above studies confirm the efficacy of electrospun phospholipid microfibers as encapsulation and antioxidant systems.

General information
State: Published
Organisations: National Food Institute, Research Group for Nano-Bio Science, Department of Chemistry, Organic Chemistry
Authors: Shekarforoush, E. (Intern), Mendes, A. C. L. (Intern), Baj, V. (Intern), Beeren, S. R. (Intern), Chronakis, I. S. (Intern)
Number of pages: 16
Publication date: 2017
Main Research Area: Technical/natural sciences
Engineering of Cellobiose Dehydrogenases for Improved Glucose Sensitivity and Reduced Maltose Affinity

Cellobiose dehydrogenase (CDH) is a fungal extracellular flavocytochrome capable of direct electron transfer (DET). Unlike other CDHs, the pH optimum for CDHs from Corynascus thermophilus (CtCDH) and Humicola insolens (HiCDH) is close to the human physiological pH in blood (7.4). These are, therefore, interesting candidates for glucose measurements in human blood and the application in enzymatic fuel cells is, however, limited by their relatively low activity with this substrate. In this work, the substrate specificities of CtCDH and HiCDH have been altered by a single cysteine to tyrosine substitution in the active sites of CtCDH (position 291) and HiCDH (position 285), which resulted in improved kinetic constants with glucose while decreasing the activity with several disaccharides, including maltose. The DET properties of the generated CDH variants were tested in the absence and in the presence of substrates, on graphite electrodes and thiolic self-assembled monolayer (SAM)-modified Au electrodes. Seven different thiols with different spacer lengths were used, containing -COOH, -OH, and -NH₂ end groups. The length and head functionality of the thiol govern the efficiency of the DET reaction and indicate different DET properties of CtCDH and HiCDH.
Engineering of Class II Cellobiose Dehydrogenases for Improved Glucose Sensitivity and Reduced Maltose Affinity

The front cover artwork is provided by Prof. Lo Gorton from Lund University (Sweden) and his co-workers. The image shows mutated cellobiose dehydrogenase (CDH) immobilized on a graphite electrode and how preferentially glucose is oxidized by this enzyme. Read the full text of the Article at 10.1002/celc.201600781.

General information
State: Published
Organisations: Department of Chemistry, Lund University, University of Natural Resources and Applied Life Sciences, Novozymes A/S
Authors: Ortiz, R. (Intern), Rahman, M. (Ekstern), Zangrilli, B. (Ekstern), Sygmund, C. (Ekstern), Micheelsen, P. O. (Ekstern), Silow, M. (Ekstern), Toscano, M. D. (Ekstern), Ludwig, R. (Ekstern), Gorton, L. (Ekstern)
Pages: 750
Publication date: 2017
Main Research Area: Technical/natural sciences

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Scopus rating (2016): CiteScore 3.77 SJR 1.499 SNIP 0.819
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.203 SNIP 0.657 CiteScore 3.13
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
BFI (2013): BFI-level 1
ISI indexed (2013): ISI indexed no
Original language: English
DOIs: 10.1002/celc.201600781
Source: Findit
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Publication: Research - peer-review › Journal article – Annual report year: 2017
Engineering Two-Dimensional Transition Metal Dichalcogenide Catalysts for Water-Splitting Hydrogen Generation

Development of advanced energy conversion and storage technologies is essential for optimizing the integration of sustainable energy resources into current-running power grid systems. As one of the key energy-storage carriers, hydrogen (H2) possesses ultrahigh gravimetric energy density, eco-friendly character and high renewability during its production and combustion processes. The development of green electricity powered H2 production techniques is a highly competitive solution to meet current energy and environmental challenges. Among different industrial approaches for H2 production, platinum supported electrocatalytic water splitting via hydrogen evolution reaction (HER) is a rather mature technique. However, it has been increasingly demanded to explore high-performance, earth-abundant and cost-effective HER electrocatalysts that can further improve energy efficiency and bring down production cost. Thanks to their abundant active edge sites, superior electrocatalytic activity, good stability and low cost, two-dimensional (2D) transition metal dichalcogenide (TMD) based electrocatalysts have been recognized as promising alternatives. This chapter deals with recent advances on the exploration of 2D-TMD based HER catalysts for water-splitting hydrogen generation. We present a brief introduction to the current main techniques for H2 production and the recent development of HER electrocatalysts. The introduction is followed by the description of the basic process of water electrolysis, general working principles of HER electrocatalysts, and main synthetic methods of 2D TMDs based materials. We then highlight some representative 2D-TMD materials used as HER electrocatalysts and conclude with the remarks and outlook of the relevant research lines.

General information
State: Published
Organisations: Department of Chemistry, NanoChemistry, Organic Chemistry
Authors: Cao, X. (Intern), Tang, Y. (Intern), Duus, J. Ø. (Intern), Chi, Q. (Intern)
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Publication date: 2017

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Editors: Martinez, L. M. T., Kharissova, O. V., Kharisov, B. I.
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ISBN (Electronic): 978-3-319-48281-1
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Bibliographical note
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Enolonium Species-Umpoled Enolates
Enolonium species/iodo(III) enolates of carbonyl compounds have been suggested to be intermediates in a wide variety of hypervalent iodine induced chemical transformations of ketones, including α-C-O, α-C-N, α-C-C, and alpha-carbon-halide bond formation, but they have never been characterized. We report that these elusive umpoled enolates may be made as
discrete species that are stable for several minutes at-78 degrees C, and report the first spectroscopic identification of such species. It is shown that enolonium species are direct intermediates in C=O, C=N, C-Cl, and C=C bond forming reactions. Our results open up chemical space for designing a variety of new transformations. We showcase the ability of enolonium species to react with prenyl, crotty, cinnamyl, and allyl silanes with absolute regioselectivity in up to 92% yield.

**General information**

State: Published
Organisations: Department of Chemistry, Ariel University Center of Samaria, Weizmann Institute of Science
Authors: Arava, S. (Ekstern), Kumar, J. N. (Ekstern), Maksymenko, S. (Ekstern), Iron, M. A. (Ekstern), Parida, K. N. (Ekstern), Fristrup, P. (Intern), Szpilman, A. M. (Ekstern)
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Scopus rating (2016): CiteScore 10.8 SJR 5.8 SNIP 2.104
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
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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
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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
Scopus rating (2008): SJR 5.438 SNIP 2.115
Web of Science (2008): Indexed yes
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 4.71 SNIP 2.119
Web of Science (2006): Indexed yes
Evaluation of equations of state for simultaneous representation of phase equilibrium and critical phenomena
Precise description of the critical points with association equations of state requires rescaling of the parameters to match experimental critical temperature and pressure of pure components. In this work we developed a method to include critical data restrictions in the parametrization procedure of the Cubic-Plus-Association (CPA) equation of state (EoS). We obtained new parameters for methanol and alkanes from n-hexane to n-decane. The comparison with the original parameters showed that this procedure is important for associating compounds, since for inert species the equation reduces to the Soave-Redlich-Kwong (SRK) EoS. The application of the rescaled parameters improved the critical point representation of pure fluids at the expense of the saturated liquid phase volume description. In the case of binary mixtures containing methanol and n-alkanes, the association model with the new parameters satisfactorily predicted the experimental critical data, indicating the importance of the rescaling parametrization procedure in the computation of the critical pressure and temperature for systems with associating species. Both sets of CPA parameters gave similar deviations in the bubble point pressure and vapor composition for the vapor-liquid equilibrium calculations. However, the rescaled parameters gave rise to larger deviations in the composition of the polar rich phase in the liquid-liquid equilibrium.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CERE – Center for Energy Ressources Engineering, Department of Chemistry
Authors: Pinto Coelho Muniz Vinhal, A. (Intern), Yan, W. (Intern), Kontogeorgis, G. (Intern)
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BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.33 SJR 0.869 SNIP 1.155
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.874 SNIP 0.998 CiteScore 1.99
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 0.982 SNIP 1.248 CiteScore 2.28
Experimental and theoretical evidence for bilayer-by-bilayer surface melting of crystalline ice

On the surface of water ice, a quasi-liquid layer (QLL) has been extensively reported at temperatures below its bulk melting point at 273 K. Approaching the bulk melting temperature from below, the thickness of the QLL is known to increase. To elucidate the precise temperature variation of the QLL, and its nature, we investigate the surface melting of hexagonal ice by combining noncontact, surfacespecific vibrational sum frequency generation (SFG) spectroscopy and spectra calculated from molecular dynamics simulations. Using SFG, we probe the outermost water layers of distinct single crystalline ice faces at different temperatures. For the basal face, a stepwise, sudden weakening of the hydrogen-bonded structure of the outermost water layers occurs at 257 K. The spectral calculations from the molecular dynamics simulations reproduce the experimental findings; this allows us to interpret our experimental findings in terms of a stepwise change from one to two molten bilayers at the transition temperature.
General information
State: Published
Organisations: Department of Chemistry, Max Planck Institute, University of Toyama, Tufts University, FOM Institute for Atomic and Molecular Physics - AMOLF, Tohoku University
Authors: Sánchez, M. A. (Intern), Kling, T. (Ekstern), Ishiyama, T. (Ekstern), van Zadel, M. (Ekstern), Bisson, P. J. (Ekstern), Mezger, M. (Ekstern), Jochum, M. N. (Ekstern), Cyran, J. D. (Ekstern), Smit, W. J. (Ekstern), Bakker, H. J. (Ekstern), Shultz, M. J. (Ekstern), Morita, A. (Ekstern), Donadio, D. (Ekstern), Nagata, Y. (Ekstern), Bonn, M. (Ekstern), Backus, E. H. G. (Ekstern)
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Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 6.767 SNIP 2.682 CiteScore 8.84
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 6.853 SNIP 2.725 CiteScore 8.86
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 6.989 SNIP 2.73 CiteScore 9.5
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 6.792 SNIP 2.682 CiteScore 9.49
ISI indexed (2012): ISI indexed yes
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BFI (2011): BFI-level 2
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ISI indexed (2011): ISI indexed yes
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BFI (2010): BFI-level 2
Scopus rating (2010): SJR 6.769 SNIP 2.529
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 6.913 SNIP 2.544
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 6.899 SNIP 2.445
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 6.766 SNIP 2.441
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 6.734 SNIP 2.434
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 6.784 SNIP 2.551
Extension of modified RAND to multiphase flash specifications based on state functions other than (T,P)

The recently proposed modified RAND formulation is extended from isothermal multiphase flash to several other state function based flash specifications. The obtained general formulation is applicable to chemical equilibrium although this study is focused on flash with only phase equilibrium. It is demonstrated that a common symmetric Jacobian matrix can be formulated for all of these flash specifications. Newton iteration with the common Jacobian is used to converge for the majority of cases and a Q-function maximisation with nested isothermal flash in the inner loop is used for the non-convergent exceptions. For isothermal flash with modified RAND, it can happen in rare occasions that the modified RAND step is ascending in the Gibbs energy. A correction of the step is proposed for such cases to obtain a descent direction without violating the condition used in the derivation of modified RAND. A two-phase example is used to demonstrate that the described method is suitable for (H,P), (T,V), (S,V) and (U,V) flash specifications and a four-phase case is examined in more detail for the difficult (U,V) case. Two- and three-phase examples close to critical regions are used to demonstrate the effectiveness of the correction procedure for the modified RAND step and to show that satisfactory rates of convergence are obtained.

General information
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Organisations: Department of Chemistry, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Ressources Engineering
Authors: Paterson, D. (Intern), Michelsen, M. L. (Intern), Yan, W. (Intern), Stenby, E. H. (Intern)
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Scopus rating (2015): SJR 0.874 SNIP 0.998 CiteScore 1.99
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
It is well known that microorganisms are surrounded by extracellular polymeric substances (EPS) which include polysaccharides, proteins, glycoproteins, nucleic acids, phospholipids, and humic acids. However, previous studies on microbial extracellular electron transfer (EET) are conducted on cells without extracting EPS or cells collected from log stage or early-steady stage cultures with little EPS. Therefore, microbial cells are believed to come in contact directly with each other or electrode. Such attempts apparently ignored the role of EPS in microbial EET, even though many components of EPS, such as DNA, humic acids, and some proteins, are electrochemically active or semiconductive. Herein, we report experimental evidences of EPS role on EET for Shewanella oneidensis MR-1. Atomic force microscopy clearly showed that the cell surface was cleaned and few EPS could be observed on MR-1 after the extraction. Comparing to cells in control group, MR-1 treated at 38 °C for EPS extraction showed different electrochemical characterizations as revealed by...
differential pulse voltammetry. EPS extracted from MR-1 also was proved to be electrochemically active. The present
study indicated that EPS play important roles in EET of MR-1.

General information
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Organisations: Department of Chemistry, NanoChemistry, Organic Chemistry, Chinese Academy of Sciences
Authors: Xiao, Y. (Intern), Zhang, J. (Intern), Ulstrup, J. (Intern), Zhao, F. (Ekstern)
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Extracellular polymeric substances are transient media for microbial extracellular electron transfer
Microorganisms exploit extracellular electron transfer (EET) in growth and information exchange with external
environments or with other cells. Every microbial cell is surrounded by extracellular polymeric substances (EPS).
Understanding the roles of three-dimensional (3D) EPS in EET is essential in microbiology and microbial exploitation for
mineral bio-respiration, pollutant conversion, and bioenergy production. We have addressed these challenges by
comparing pure and EPS-depleted samples of three representative electrochemically active strains viz Gram-negative
Shewanella oneidensis MR-1, Gram-positive Bacillus sp. WS-XY1, and yeast Pichia stipites using technology from
electrochemistry, spectroscopy, atomic force microscopy, and microbiology. Voltammetry discloses redox signals from
cytochromes and flavins in intact MR-1 cells, whereas stronger signals from cytochromes and additional signals from both
flavins and cytochromes are found after EPS depletion. Flow cytometry and fluorescence microscopy substantiated by N-
acetylglucosamine and electron transport system activity data showed less than 1.5% cell damage after EPS extraction.
The electrochemical differences between normal and EPS-depleted cells therefore originate from electrochemical species
in cell walls and EPS. The 35 ± 15-nm MR-1 EPS layer is also electrochemically active itself, with cytochrome electron
transfer rate constants of 0.026 and 0.056 s⁻¹ for intact MR-1 and EPS-depleted cells, respectively. This surprisingly small
rate difference suggests that molecular redox species at the core of EPS assist EET. The combination of all the data with
electron transfer analysis suggests that electron "hopping" is the most likely molecular mechanism for electrochemical
electron transfer through EPS.

General information
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Organisations: Department of Chemistry, NanoChemistry, Organic Chemistry, Metalloprotein Chemistry and Engineering,
Chinese Academy of Sciences, Hunan University
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M. (Intern), Ulstrup, J. (Intern), Zhao, F. (Ekstern)
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Fabricating interstitial-free steel with simultaneous high strength and good ductility with homogeneous layer and lamella structure

Annealed interstitial-free steel (IF steel) and deformed IF steel sheets were stacked alternatively into multi-layers to produce laminated IF steel through thermal-mechanical processing. After proper processing, a yield strength of 500 MPa, an ultimate tensile strength of 600 MPa (comparable to cold rolled one) and a uniform elongation around 17% can be realized. Microstructural observation by electron back-scatter diffraction revealed a characteristic hierarchical layer + heterogeneous lamella structure, namely L2 structure. The reasons for the good mechanical properties were discussed.

General information
State: Published
Organisations: Department of Chemistry, NanoChemistry, Department of Wind Energy, Materials science and characterization, Chongqing University, Yanshan University
Authors: Zhang, L. (Intern), Chen, Z. (Ekstern), Wang, Y. (Ekstern), Ma, G. (Ekstern), Huang, T. (Ekstern), Wu, G. (Ekstern), Juul Jensen, D. (Intern)
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Scopus rating (2016): CiteScore 3.71 SJR 1.901 SNIP 1.696
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Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.744 SNIP 2.124 CiteScore 3.55
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.347 SNIP 1.975 CiteScore 3.19
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 2.309 SNIP 2.022 CiteScore 3.01
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 2.333 SNIP 2.108 CiteScore 3.21
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 2.445 SNIP 2.125
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.574 SNIP 2.02
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 2.634 SNIP 2.128
Web of Science (2008): Indexed yes
Facile and Benign Conversion of Sucrose to Fructose Using Zeolites With Balanced Brønsted and Lewis Acidity

Sucrose is by far the industrially most abundant simple carbohydrate with a production volume of more than 160 million metric tons from sugar cane and sugar beet per year. Many promising pathways towards bio-based organic compounds use, however, fructose as the pathway substrate. Hence, a chemocatalytic approach to convert sucrose into fructose would provide a means to channel sucrose into pathways for sugar valorization. Here, we show that a variety of heterogeneous zeolite catalysts with balanced Brønsted and Lewis acidity enable a simple route for the conversion of sucrose to more than 80% fructosides or fructose at 100 °C. The catalysts can encompass aluminum or tin Lewis acidic sites in various zeolite frameworks. The reaction proceeds in volatile alcohol solvents and broadly enables the channelling of sucrose into processes that use fructose as the pathway substrate.
Femtochemistry in the electronic ground state: Dynamic Stark control of vibrational dynamics

We study the interplay of vibrational and rotational excitation in a diatomic molecule due to the non-resonant dynamic Stark effect. With a fixed peak intensity, optimal Gaussian pulse durations for maximizing vibrational or rotational transitions are obtained analytically and confirmed numerically for the H₂ and Cl₂ molecules. In general, pulse trains or more advanced pulse shaping techniques are required in order to obtain significant vibrational excitation. To that end, we demonstrate that a high degree of selectivity between vibrational and rotational excitation is possible with a suitably phase-modulated Gaussian pulse.
Fe$_3$O$_4$@polyaniline yolk–shell micro/nanospheres as bifunctional materials for lithium storage and electromagnetic wave absorption

Unique Fe$_3$O$_4$/polyaniline (PANI) composite with yolk-shell micro/nanostructure (FPys) has been successfully synthesized by a facile silica-assisted in-situ polymerization and subsequent etching strategy. The structural and compositional studies of the FPys composites are performed by employing X-ray diffraction (XRD), and X-ray photoelectron spectroscopy (XPS). The yolk-shell morphology of the products is confirmed by scanning electron microscopy (SEM) and transmission electron microscopy (TEM) observations. When evaluated as anode material for lithium-ion batteries, the as-prepared FPys electrodes deliver superior capacity, better cycling stability and rate capability than those of bare Fe$_3$O$_4$ micro/nanospheres and Fe$_3$O$_4$/PANI core-shell (FPcs) electrodes. Moreover, FPys also exhibits excellent electromagnetic wave absorption performance when comparing to the synthesized Fe$_3$O$_4$-based electromagnetic wave absorbers, in which strong reflection loss and extensive response bandwidth can be achieved simultaneously. The excellent bifunctional properties of FPys material are associated with the specially designed hierarchical micro/nanostructures. The current strategy that application directed structural design can be applied to the synthesis of other multifunctional materials.

General information
State: Published
Organisations: Department of Chemistry, NanoChemistry, Organic Chemistry, Department of Micro- and Nanotechnology, Molecular Windows, Hebei University of Science and Technology, Central South University
Authors: Wang, X. (Ekstern), Zhang, M. (Intern), Zhao, J. (Intern), Huang, G. (Ekstern), Sun, H. (Intern)
Pages: 1054-1063
Flexible, lightweight and paper-like supercapacitors assembled from nitrogen-doped multi-dimensional carbon materials

Flexible supercapacitors have shown great potential to fulfill the increasing demand on wearable, miniature, lightweight, thin and highly efficient power supply systems for advanced portable electronics. Owing to its superior supercapacitive performances as well as high chemical stability and excellent mechanical flexibility, graphene (GR) based flexible supercapacitors have received much research attention in recent years. However, GR-based supercapacitors often suffer from GR restacking leading to capacitance attenuation. Therefore, some macromolecules, polymers and zero-dimensional/one-dimensional (00/10) nanomaterials have been tested as spacers to prevent GR sheets (GRSs) from restacking for constructing three-dimensional (30) porous electrodes. Besides, heteroatom doping of GRSs could further improve their specific capacitance by introducing pseudocapacitive characteristics and increasing hydrophilicity. In this work, a facile approach is developed to prepare nitrogen-doped carbon based flexible and free-standing paper electrodes (N3CPs) built from three types of representative carbon materials in different dimensions (0D: carbon black nanoparticles (CBNPs); 10: carbon nanotubes (CNTs); 20: GRSs) with melamine as the nitrogen doping source. The N3CP electrode has demonstrated several advantages, such as enhanced porosity, improved electrical conductivity and high nitrogen doping level. Electrochemical tests have shown that thanks to the synergistic effects of hybrid-dimensional optimized carbon materials, 30 hierarchical porous nanostructure and effective nitrogen doping, a N3CP based flexible supercapacitor has shown the combined advantages of high capacitance, high rate capability and long cycling life (>20,000 cycles). The results hold promising prospects towards practical applications of such flexible supercapacitors in portable electronics.

Flooding of North Sea chalk and greensand cores with specific brines

Flooding of North Sea chalk and greensand cores with specific brines
Freestanding and flexible graphene papers as bioelectrochemical cathode for selective and efficient CO₂ conversion

During microbial electrosynthesis (MES) driven CO₂ reduction, cathode plays a vital role by donating electrons to microbe. Here, we exploited the advantage of reduced graphene oxide (RGO) paper as novel cathode material to enhance electron transfer between the cathode and microbe, which in turn facilitated CO₂ reduction. The acetate production rate of Sporomusa ovata-driven MES reactors was 168.5 ± 22.4 mmol m⁻² d⁻¹ with RGO paper cathodes poised at −690 mV versus standard hydrogen electrode. This rate was approximately 8 fold faster than for carbon paper electrodes of the same dimension. The current density with RGO paper cathodes of 2580 ± 540 mA m⁻² was increased 7 fold compared to carbon paper cathodes. This also corresponded to a better cathodic current response on their cyclic voltammetric curves. The coulombic efficiency for the electrons conversion into acetate was 90.7 ± 9.3% with RGO paper cathodes and 83.8 ± 4.2% with carbon paper cathodes, respectively. Furthermore, more intensive cell attachment was observed on RGO paper electrodes than on carbon paper electrodes with confocal laser scanning microscopy and scanning electron microscopy. These results highlight the potential of RGO paper as a promising cathode for MES from CO₂.

General information
State: Published
Organisations: Novo Nordisk Foundation Center for Biosustainability, Research Groups, Department of Chemistry, NanoChemistry, Department of Micro- and Nanotechnology, Nanocarbon, Organic Chemistry
Authors: Aryal, N. (Intern), Halder, A. (Intern), Zhang, M. (Intern), Whelan, P. R. (Intern), Tremblay, P. (Intern), Chi, Q. (Intern), Zhang, T. (Intern)
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Scopus rating (2016): CiteScore 4.63 SJR 1.625 SNIP 1.401
Web of Science (2015): Indexed yes
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Web of Science (2015): Indexed yes
Scopus rating (2015): SJR 2.057 SNIP 1.684 CiteScore 5.3
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BFI (2014): BFI-level 1
Web of Science (2014): Indexed yes
Scopus rating (2014): SJR 2.103 SNIP 1.544 CiteScore 4.75
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Web of Science (2013): Indexed yes
Scopus rating (2013): SJR 1.886 SNIP 1.51 CiteScore 4.06
ISI indexed (2013): ISI indexed yes
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BFI (2012): BFI-level 1
Web of Science (2012): Indexed yes
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Functional and structural characterization of plastidic starch phosphorylase during barley endosperm development

The production of starch is essential for human nutrition and represents a major metabolic flux in the biosphere. The biosynthesis of starch in storage organs like barley endosperm operates via two main pathways using different substrates: starch synthases use ADP-glucose to produce amylose and amylopectin, the two major components of starch, whereas starch phosphorylase (Pho1) uses glucose-1-phosphate (G1P), a precursor for ADP-glucose production, to produce α-1,4 glucans. The significance of the Pho1 pathway in starch biosynthesis has remained unclear. To elucidate the importance of barley Pho1 (HvPho1) for starch biosynthesis in barley endosperm, we analyzed HvPho1 protein production and enzyme activity levels throughout barley endosperm development and characterized structure-function relationships of HvPho1. The molecular mechanisms underlying the initiation of starch granule biosynthesis, that is, the enzymes and substrates involved in the initial transition from simple sugars to polysaccharides, remain unclear. We found that HvPho1 is present as an active protein at the onset of barley endosperm development. Notably, purified recombinant protein can catalyze the de novo production of α-1,4-glucans using HvPho1 from G1P as the sole substrate. The structural properties of HvPho1 provide insights into the low affinity of HvPho1 for large polysaccharides like starch or amylpectin. Our results suggest that HvPho1 may play a role during the initiation of starch biosynthesis in barley.

General information
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Organisations: Department of Chemistry, Organic Chemistry, Department of Biotechnology and Biomedicine, Enzyme and Protein Chemistry, Carlsberg Research Laboratory, Virginia Polytechnic Institute and State University
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Scopus rating (2016): CiteScore 3.11 SJR 1.201 SNIP 1.092
Web of Science (2016): Indexed yes
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Scopus rating (2015): SJR 1.414 SNIP 1.131 CiteScore 3.32
Web of Science (2015): Indexed yes
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Scopus rating (2014): SJR 1.545 SNIP 1.141 CiteScore 3.54
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.74 SNIP 1.147 CiteScore 3.94
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.945 SNIP 1.142 CiteScore 4.15
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.369 SNIP 1.23 CiteScore 4.58
ISI indexed (2011): ISI indexed no
Web of Science (2011): Indexed yes
Fungi & Health: can polysaccharides from the fungus inonotus obliquus (CHAGA) inhibit tumor growth?

Inonotus obliquus (Chaga) – a white rot fungus found on birch trees in the northern hemisphere – has been used in traditional medicine in Europe and Asia for centuries. Native peoples have made use of Chaga by brewing it as a tea to treat gastrointestinal problems, to heal wounds and even to treat cancer. The last few decades, studies have found Chaga to contain biologically active substances such as polysaccharides, triterpenoids, polyphenols and melanin. In vivo effects such as tumor growth inhibition have been observed in mice receiving various Chaga extracts. The main hypothesis behind the tumor inhibiting effect is two-fold: i) fungal polysaccharides may inhibit tumor growth indirectly by activating certain immune cells such as macrophages and ii) triterpenoids and other steroids from Chaga may give a direct cytotoxic effect against cancer cells. While triterpenoids from Chaga have been extensively characterized, detailed analysis of the polysaccharides is lacking. The present work has aimed to isolate and characterize the polysaccharides in Chaga, by e.g. column chromatography (ionexchange/gel filtration), GC-MS, SEC-MALLS and extensive NMR analysis. The water-soluble polysaccharides were found to be complex hetero-polysaccharides, with a structure dominated by(1→3/1→6)-β-glucan and (1→6)-α-galactan, with β-xylose, α-mannose and α-galacturonic acid present in significant amounts. 3-O-methyl α-galactose was reported in Chaga for the first time. The polysaccharide fractions obtained were screened in in vitro bioassays for their potential as immunomodulators. Several fractions showed promising results by activating murine bone marrow derived macrophages to inhibit the growth of Lewis lung carcinoma cells in vitro. The results suggest further studies to be conducted on immune cell activation and in vivo tumor growth inhibition.

General information

State: Published
Organisations: Department of Chemistry, Organic Chemistry, University of Oslo, Oslo University Hospital, Norwegian University of Science and Technology
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Main Research Area: Technical/natural sciences
Electronic versions: LIBRO_COMPLETO_EUROCARB10.pdf
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General approach to characterizing reservoir fluids for EoS models using a large PVT database

Fluid characterization is needed when applying any EoS model to reservoir fluids. It is important especially for non-cubic models such as PC-SAFT where fluid characterization is less mature. Furthermore, there is a great interest to apply non-cubic models to high pressure high temperature reservoir fluids as they are believed to give better description of density and compressibility over a wide temperature and pressure range. We proposed a general approach to characterizing reservoir fluids and applied it to PC-SAFT. The approach consists in first, developing the correlations based on the DIPPR database, and then adjusting the correlations based on a large PVT database. The adjustment was made to minimize the
deviation in key PVT properties like saturation pressures, densities at reservoir temperature and stock tank oil densities, while keeping the n-alkane limit of the correlations unchanged. The general approach can also be applied to other EoS models for improving their fluid characterization and we showed this for SRK and PR. In addition, we developed a PNA based characterization method for PC-SAFT based on the same general principles. We made a comprehensive comparison in PVT calculation involving 17 EoS-characterization combinations and 260 reservoir fluids. The new characterization methods generally improved the PVT calculation results.

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Organisations: Department of Chemistry, Center for Energy Resources Engineering, CERE – Center for Energy Resources Engineering
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Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.33 SJR 0.869 SNIP 1.155
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.874 SNIP 0.998 CiteScore 1.99
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 0.982 SNIP 1.248 CiteScore 2.28
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.007 SNIP 1.274 CiteScore 2.31
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.152 SNIP 1.286 CiteScore 2.31
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.034 SNIP 1.234 CiteScore 2.26
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 0.986 SNIP 1.317
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.133 SNIP 1.164
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.227 SNIP 1.09
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.031 SNIP 1.151
N-Aryl-1,1,1-trichloromethanesulfenamides ArNH-SCl3 easily undergo dehydrochlorination upon treatment with potassium hydroxide in ethanolic solution. The intermediate thiocarbonyl S-imides formed thereby behave differently depending on the type of the N-aryl group. The sterically crowded N-(2,6-dimethylphenyl)- and -N-(2,4,6-trimethylphenyl)-1,1,1-trichloromethanesulfenamides yield the corresponding sulfur N,N’-diaryldiimides via a multi-step reaction, whereas the less crowded 2-methylphenyl and 4-methylphenyl derivatives undergo a regioselective 'head-to-head' dimerization leading to 5,5,6,6-tetrachloro-1,4,2,3-dithiadiazinanes in high yields. An identical reaction course is observed in the case of the 4-methoxy- and 4-bromoaniline derivatives. A diradical mechanism is postulated to explain the 'head-to-head' dimerization pathway.
Giant tunability of the two-dimensional electron gas at the interface of γ-Al₂O₃/SrTiO₃

Two-dimensional electron gases (2DEGs) formed at the interface between two oxide insulators provide a rich platform for the next generation of electronic devices. However, their high carrier density makes it rather challenging to control the interface properties under a low electric field through a dielectric solid insulator, i.e. in the configuration of conventional field-effect transistors. To surpass this long-standing limit, we used ionic liquids as the dielectric layer for electrostatic gating of oxide interfaces in an electric double layer transistor (EDLT) configuration. Herein, we reported giant tunability of the physical properties of 2DEGs at the spinel/perovskite interface of γ-Al₂O₃/SrTiO₃ (GAO/STO). By modulating the carrier density thus the band filling with ionic-liquid gating, the system experiences a Lifshitz transition at a critical carrier density of 3.0×10¹³ cm⁻², where a remarkably strong enhancement of Rashba spin-orbit interaction and an emergence of Kondo effect at low temperatures are observed. Moreover, as the carrier concentration depletes with decreasing gating voltage, the electron mobility is enhanced by more than 6 times in magnitude, leading to the observation of clear quantum oscillations. The great tunability of GAO/STO interface by EDLT gating not only shows promise for design of oxide devices with on-demand properties, but also sheds new light on the electronic structure of 2DEG at the non-isostructural spinel/perovskite interface.

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Global phylogenetic analysis of contemporary aleutian mink disease viruses (AMDVs)

Aleutian mink disease has major economic consequences on the mink farming industry worldwide, as it causes a disease that affects both the fur quality and the health and welfare of the mink. The virus causing this disease is a single-stranded DNA virus of the genus Amdparvovirus belonging to the family of Parvoviridae. In Denmark, infection with AMDV has largely been restricted to a region in the northern part of the country since 2001, affecting only 5% of the total Danish mink farms. However, in 2015 outbreaks of AMDV were diagnosed in all parts of the country. Initial analyses revealed that the outbreaks were caused by two different strains of AMDV that were significant different from the circulating Danish strains. To track the source of these outbreaks, a major investigation of global AMDV strains was initiated. Samples from 13 different countries were collected and partial NS1 gene was sequenced and subjected to phylogenetic analyses. The analyses revealed that AMDV exhibited substantial genetic diversity. No clear country wise clustering was evident, but exchange of viruses between countries was revealed. One of the Danish outbreaks was caused by a strain of AMDV that closely resembled a strain originating from Sweden. In contrast, we did not identify any potential source for the other and more widespread outbreak strain. To the authors knowledge this is the first major global phylogenetic study of contemporary AMDV partial NS1 sequences. The study proved that partial NS1 sequencing can be used to distinguish virus strains belonging to major clusters. The partial NS1 sequencing can therefore be a helpful tool in combination with epidemiological data, in relation to outbreak tracking. However detailed information on farm to farm transmission requires
full genome sequencing.

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Scopus rating (2015): SJR 1.185 SNIP 0.947 CiteScore 2.47
Scopus rating (2014): SJR 1.044 SNIP 0.911 CiteScore 2.27
Web of Science (2014): Indexed yes
Scopus rating (2013): SJR 1.031 SNIP 0.981 CiteScore 2.44
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Scopus rating (2012): SJR 0.957 SNIP 0.866 CiteScore 2.37
ISI indexed (2012): ISI indexed yes
Scopus rating (2011): SJR 1.057 SNIP 0.9 CiteScore 2.65
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
Scopus rating (2010): SJR 1.071 SNIP 0.865
Web of Science (2010): Indexed yes
Scopus rating (2009): SJR 0.986 SNIP 0.754
Scopus rating (2008): SJR 0.618 SNIP 0.537
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.6 SNIP 0.562
Web of Science (2007): Indexed yes
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Scopus rating (2005): SJR 0.391 SNIP 0.358
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Glucagon-like Peptide 1 Conjugated to Recombinant Human Serum Albumin Variants with Modified Neonatal Fc Receptor Binding Properties. Impact on Molecular Structure and Half-Life
Glucagon-like peptide 1 (GLP-1) is a small incretin hormone stimulated by food intake, resulting in an amplification of the insulin response. Though interesting as a drug candidate for the treatment of type 2 diabetes mellitus, its short plasma
half-life of less than 3 minutes limits its clinical use. A strategy to extend the half-life of GLP-1 utilizes the long half-life of human serum albumin (HSA) by combining the two via chemical conjugation or genetic fusion. HSA has a plasma half-life of around 21 days owing to its interaction with the neonatal Fc receptor (FcRn) expressed in endothelial cells of blood vessels, which rescues circulating HSA from lysosomal degradation. We have conjugated GLP-1 to C34 of native sequence recombinant HSA (rHSA) and two rHSA variants; one with increased and one with decreased binding affinity to hFcRn. We have investigated the impact of conjugation on FcRn binding affinities, GLP-1 potency and pharmacokinetics, combined with the solution structure of the rHSA variants and GLP-1 albumin conjugates. The solution structures, determined by small angle X-ray scattering, show the GLP-1 pointing away from the surface of rHSA. Combining the solution structures with the available structural information on the FcRn and GLP-1 receptor (GLP-1R) obtained from X-ray crystallography, we can explain the observed in-vitro and in-vivo behaviour. We conclude that the conjugation of GLP-1 to rHSA does not affect the interaction between rHSA and FcRn, while the observed decrease in the potency of GLP-1 can be explained by a steric hindrance of GLP-1 binding to its receptor.
Glucose Isomerization by Enzymes and Chemo-catalysts: Status and Current Advances

The well-known interconversion of aldoses to their corresponding ketoses was discovered more than a century ago, but has recently attracted renewed attention due to alternative application areas. Since the pioneering discovery, much work has been directed toward improving the process of isomerization of aldoses in terms of yields, catalysts, solvents, catalytic systems, etc., by both enzymatic and chemo-catalytic approaches. Among aldose ketose interconversion reactions, fructose production by glucose isomerization to make high-fructose corn syrup (HFCS) is an industrially important and large biocatalytic process today, and a large number of studies have been reported on the process development. In parallel, also alternative chemo-catalytic systems have emerged, as enzymatic conversion has drawbacks, though they are typically more selective and produce fructose under mild reaction conditions. Isomerization of glucose is also a central reaction for making renewable platform chemicals, such as lactic acid, 5-hydroxymethylfurfural (HMF), and levulinic acid. In these other applications, thermally stable catalysts are required, thus making use of enzymatic catalysis inadequate, since enzymes generally possess a limited temperature operating window, typically less than 80 ºC. From this viewpoint, the chemo-catalysts especially solid heterogeneous catalysts are playing a key role for the development of not only making HFCS, but also making chemicals and fuels from glucose via the isomerized product/intermediate fructose. This review focuses on how both enzyme and chemo-catalysts are being useful for the isomerization of glucose to fructose. Specifically, development of Lewis acid containing zeolites for glucose isomerization is reviewed in detail, including mechanism, isotopic labeling, and computational studies.

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry, Guizhou University, Center of Innovative and Applied Bioprocessing
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Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 10.3 SJR 4.299 SNIP 2.071
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 4.039 SNIP 2.134 CiteScore 9.88
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 3.641 SNIP 2.022 CiteScore 8.74
Web of Science (2014): Indexed yes
Graphene-Conducting Polymer Nanocomposites for Enhancing Electrochemical Capacitive Energy Storage

The evolution of power generation, expansion of transportation and electrification, and popularization of portable electronic devices have altogether posed growing demands for more efficient energy storage systems. Supercapacitors, as one of major electrochemical energy storage devices, have recently received intensive attention. In this minireview, our focus is on graphene-conducting polymer nanocomposites and their applications in supercapacitors that have potential to perform high power and energy density, fast charge/discharge rate, low cost and eco-friendly operation conditions. We first introduce major types of supercapacitors and their working principles. We then overview several hybrid material systems combing graphene and various conducting polymers such as polyaniline, polythiophene, polypyrrole and their derivatives, with the emphasis on the composite design, synthesis methods, capacitive performance and current applications in flexible and bendable supercapacitors. Finally, the challenges and perspective of such composite electrode materials for supercapacitors are commented for perspective of further research directions.

General information
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Organisations: Department of Chemistry, NanoChemistry, Organic Chemistry
Authors: Shen, F. (Intern), Pankratov, D. (Intern), Chi, Q. (Intern)
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Graphene directed architecture of fine engineered nanostructures with electrochemical applications

Thanks to its high performance as a conducting or/and chemically active support material, graphene has offered unique opportunities for developing novel nanostructured materials to meet various demands. The assembly of graphene with other nanoscale building blocks such as metals, metal oxides, and polymers has led to the possibility to create new electroactive and multifunctional nanostructures, which can serve as promising material platforms for electrochemical purposes. However, the precise control and fine-tuning of material structures and properties are still challenging and in demand. In this review, we aim to highlight some recent efforts devoted to rational design, assembly and fine engineering of electrochemically active nanostructures using graphene or/and its derivatives as soft templates for controlled synthesis and directed growth. We organize the contents according to the chemically classified nanostructures, including metallic nanostructures, self-assembled organic and supramolecular structures, and fine engineered metal oxides. In these cases, graphene templates either sacrificed during templating synthesis or retained as support for final products. We also discuss remained challenges and future perspective in the graphene-templating design and synthesis of various materials. Overall, this review could offer crucial insights into the nanoscale engineering of new nanostructures using graphene as a soft template and their potential applications in electrochemical science and technology. We hope this review would also
stimulate new ideas and approaches for relevant ongoing research.

**General information**

State: Published
Organisations: Department of Chemistry, NanoChemistry, Department of Micro- and Nanotechnology, Organic Chemistry
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- Web of Science (2017): Indexed yes
- BFI (2016): BFI-level 2
- Scopus rating (2016): CiteScore 4.74 SJR 1.357 SNIP 1.167
- Web of Science (2016): Indexed yes
- BFI (2015): BFI-level 2
- Scopus rating (2015): SJR 1.349 SNIP 1.344 CiteScore 4.86
- Web of Science (2015): Indexed yes
- BFI (2014): BFI-level 2
- Scopus rating (2014): SJR 1.391 SNIP 1.482 CiteScore 4.59
- Web of Science (2014): Indexed yes
- BFI (2013): BFI-level 1
- Scopus rating (2013): SJR 1.435 SNIP 1.607 CiteScore 4.44
- ISI indexed (2013): ISI indexed yes
- Web of Science (2013): Indexed yes
- BFI (2012): BFI-level 1
- Scopus rating (2012): SJR 1.651 SNIP 1.592 CiteScore 3.99
- ISI indexed (2012): ISI indexed yes
- Web of Science (2012): Indexed yes
- BFI (2011): BFI-level 1
- Scopus rating (2011): SJR 1.621 SNIP 1.803 CiteScore 4.15
- ISI indexed (2011): ISI indexed yes
- Web of Science (2011): Indexed yes
- BFI (2010): BFI-level 1
- Scopus rating (2010): SJR 1.691 SNIP 1.725
- Web of Science (2010): Indexed yes
- BFI (2009): BFI-level 1
- Scopus rating (2009): SJR 1.536 SNIP 1.625
- BFI (2008): BFI-level 1
- Scopus rating (2008): SJR 1.533 SNIP 1.47
- Web of Science (2008): Indexed yes
- Scopus rating (2007): SJR 1.563 SNIP 1.595
- Web of Science (2007): Indexed yes
- Scopus rating (2006): SJR 1.534 SNIP 1.736
- Web of Science (2006): Indexed yes
- Scopus rating (2005): SJR 1.481 SNIP 1.533
- Web of Science (2005): Indexed yes
- Scopus rating (2004): SJR 1.365 SNIP 1.581
- Scopus rating (2003): SJR 1.628 SNIP 1.526
Graphene-encapsulated Fe₃O₄ nanorods assembled into a mesoporous hybrid composite used as a high-performance lithium-ion battery anode material

The discovery of new anode materials and engineering their fine structures are the core elements in the development of new-generation lithium-ion batteries (LIBs). To this end, we herein report a novel nanostructured composite consisting of approximately 75% Fe₃O₄ nanorods and 25% reduced graphene oxide (rGO). Microscopy and spectroscopy analyses have identified that the Fe₃O₄ nanorods are wrapped (or encapsulated) by the rGO nanosheets via covalent bonding, which further self-assemble into a mesoporous hybrid composite networked by the graphene matrix. The composite has an average pore size around 20 nm and exhibits a high surface area of 152 m² g⁻¹, which is 76 times as high as that of conventional Fe₃O₄ powder. We have used the composite as an LIB anode material to fabricate coin-type prototype cells with lithium as the cathode. Systematic half-cell testing evaluations show that the electrochemical performance of the present composite material is amongst the best of the transition metal-oxide based LIB anode materials. The performances are characterized by a high reversible capacity of 1053 mA h g⁻¹ subjected to 250 charge–discharge cycles at 500 mA g⁻¹ and an excellent rate capability with the deliverable energy of 786–541 mA h g⁻¹ upon the application of high current densities of 1000–5000 mA g⁻¹. Overall, we have demonstrated that Fe₃O₄ nanorod–rGO hybrid composite is an interesting and promising material for the fabrication of LIB anodes.

Graphene-glucose oxidase bioanodes for enzymatic biofuel cells

Enzymatic biofuel cells (EBFCs) are electrochemical devices, that produce electricity from energy stored in fuel molecules under catalysis of enzymes. An EBFC contains a bioanode and/or a biocathode, in which enzymes are used to catalyse oxidation of fuel molecules such as sugars, and dioxygen reduction, respectively. The advantage of EBFCs is to generate energy from abundant fuel molecules without using expensive noble metals. On the other hand, development of EBFCs is still at the research stage due to instability of the biocatalysts. Here, we are developing a bioanode using graphene as supporting material, polyethyleneimine (PEI) as linker and glucose oxidase (GOD) as the chosen enzyme. GOD can catalyze oxidation of glucose to gluconolactone, but needs a mediator to assist electron transfer between the enzyme and
electrodes. The redox molecule ferrocene carboxylic acid (FcCOOH) is immobilized together with GOD on the bioanode. Structure and composition of the graphene-GOD bioanode are shown in Fig. 1b. Electrochemical catalytic performance of the prepared bioanode has been observed. An EBFCs with the bioanode and the commercial Pt cathode have been successfully assembled and systematically investigated. The assembled EBFCs show good reproducibility. EBFCs provide maximum output power density 2.47 μW cm⁻² at 35 ℃, indicating the optimized activity of EBFCs fed with glucose.

Graphene-Paper Based Electrochemical Sensors
Graphene paper as a new form of graphene-supported nanomaterials has received worldwide attention since its first report in 2007. Due to their high flexibility, lightweight and good electrical conductivity, graphene papers have demonstrated the promising potential for crucial applications in electrochemical sensors and energy technologies amongst others. In this chapter, we present some examples to overview recent advances in the research and development of two-dimensional (2D) graphene papers as new materials for electrochemical sensors. The chapter covers the design, fabrication, functionalization and application evaluations of graphene papers. We first summarize the mainstream methods for fabrication of graphene papers/membranes, with the focus on chemical vapour deposition techniques and solution-processing assembly approaches. A large portion of this chapter is then devoted to the highlights of specific functionalization of graphene papers with polymer and nanoscale functional building blocks for electrochemical-sensing purposes. In terms of electrochemical-sensing applications, the emphasis is on enzyme-graphene and nanoparticle-graphene paper-based systems for the detection of glucose. We finally conclude this chapter with brief remarks and outlook.

Bibliographical note
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Graphene papers: smart architecture and specific functionalization for biomimetics, electrocatalytic sensing and energy storage

Paper is an attractively assembled form of materials and has accompanied our daily life almost everywhere. Two-dimensional layered materials, especially graphene, have unique intrinsic structures to be exploited for smart architecture of macroscopic papers that are offering many newly emerging applications. Research advances in graphene based papers in the past few years have created a new category of composite materials. This review aims at offering an up-to-date comprehensive summary of graphene-supported papers, with the emphasis on smart assembly and purpose-driven specific functionalization for their critical applications associated with sensing, environmental and energy technologies. The contents of this review are based on a balance combination of our own studies and selected research studies done by worldwide academic groups. We first give a brief introduction to graphene as a versatile building block and to the current status of research studies on graphene papers. This is followed by addressing some crucial methods of how to prepare graphene papers. We then summarize multiple possibilities of functionalizing graphene papers, membranes or films. Finally, we evaluate some key applications of graphene papers in the areas of chemical/electrochemical sensors, biomimetics and energy storage devices, just before leading to our concluding remarks and perspectives.

General information
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Organisations: Department of Chemistry, NanoChemistry, Organic Chemistry, Donghua University
Authors: Zhang, M. (Intern), Hou, C. (Intern), Halder, A. (Intern), Wang, H. (Ekstern), Chi, Q. (Intern)
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Grid-Based Projector Augmented Wave (GPAW) Implementation of Quantum Mechanics/Molecular Mechanics (QM/MM)
Electrostatic Embedding and Application to a Solvated Diplatinum Complex

A multiscale density functional theory-quantum mechanics/molecular mechanics (DFT-QM/MM) scheme is presented, based on an efficient electrostatic coupling between the electronic density obtained from a grid-based projector augmented wave (GPAW) implementation of density functional theory and a classical potential energy function. The scheme is implemented in a general fashion and can be used with various choices for the descriptions of the QM or MM regions. Tests on H2O clusters, ranging from dimer to decamer show that no systematic energy errors are introduced by the coupling that exceeds the differences in the QM and MM descriptions. Over 1 ns of liquid water, Born-Oppenheimer QM/MM molecular dynamics (MD) are sampled combining 10 parallel simulations, showing consistent liquid water structure over the QM/MM border. The method is applied in extensive parallel MD simulations of an aqueous solution of the diplatinum [Pt2(P2O5H2)4]4- complex (PtPOP), spanning a total time period of roughly half a nanosecond. An average Pt-Pt distance deviating only 0.01 Å from experimental results, and a ground-state Pt-Pt oscillation frequency deviating by

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Heat capacity and Joule-Thomson coefficient of selected n-alkanes at 0.1 and 10 MPa in broad temperature ranges

Isobaric heat capacity of six n-alkanes, i.e. n-hexane, n-octane, n-decane, n-dodecane, n-tetradecane and n-hexadecane, was determined with a Calvet type differential heat-flux calorimeter at 0.1 and 10 MPa in a broad temperature range. The measured isobaric heat capacity data were combined with the literature density data for these n-alkanes to determine the corresponding Joule-Thomson coefficients. Four different EoSs, Soave-Redlich-Kwong, Peng-Robinson, Perturbed Chain Statistical Associating Fluid Theory, and Soave-Benedict-Webb-Rubin, were used to model the heat capacities and Joule-Thomson coefficients. Moreover, the Joule-Thomson inversion curves for these n-alkanes were also calculated by the four EoSs.

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State: Published
Organisations: Department of Chemistry
Authors: Regueira Muñiz, T. (Intern), Varzandeh, F. (Intern), Stenby, E. H. (Intern), Yan, W. (Intern)
Pages: 250-264
Publication date: 2017
Main Research Area: Technical/natural sciences
Publication information
Journal: Journal of Chemical Thermodynamics
Volume: 111
ISSN (Print): 0021-9614
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.64 SJR 1 SNIP 1.163
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.075 SNIP 1.091 CiteScore 2.29
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.224 SNIP 1.306 CiteScore 2.59
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.252 SNIP 1.25 CiteScore 2.42
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.221 SNIP 1.181 CiteScore 2.41
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.24 SNIP 1.307 CiteScore 2.44
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.218 SNIP 1.462
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.116 SNIP 1.355
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.414 SNIP 1.269
Scopus rating (2007): SJR 1.264 SNIP 1.176
Scopus rating (2006): SJR 1.116 SNIP 1.415
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.913 SNIP 1.277
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.847 SNIP 1.124
Scopus rating (2003): SJR 0.726 SNIP 0.986
Scopus rating (2002): SJR 0.712 SNIP 1.21
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.581 SNIP 0.984
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 0.741 SNIP 1.164
Scopus rating (1999): SJR 0.914 SNIP 1.163
Original language: English
n-alkane, Heat capacity, Joule-Thomson coefficient, High pressure, High temperature
DOIs:
10.1016/j.jct.2017.03.034
Source: PublicationPreSubmission
Source-ID: 131007722
Heme isomers substantially affect heme’s electronic structure and function

Inspection of heme protein structures in the protein data bank reveals four isomers of heme characterized by different relative orientations of the vinyl side chains; remarkably, all these have been reported in multiple protein structures. Density functional theory computations explain this as due to similar energy of the isomers but with a sizable (25 kJ mol\(^{-1}\)) barrier to interconversion arising from restricted rotation around the conjugated bonds. The four isomers, EE, EZ, ZE, and ZZ, were then investigated as 4-coordinate hemes, as 5-coordinate deoxyhemes, in 6-coordinate \(\text{O}_2\)-adducts of globins and as compound I intermediates typical of heme peroxidases. Substantial differences were observed in electronic properties relevant to heme function: notably, the spin state energy gap of \(\text{O}_2\)-heme adducts, important for fast reversible binding of \(\text{O}_2\), depends on the isomer state, and \(\text{O}_2\)-binding enthalpies change by up to 16 kJ mol\(^{-1}\); redox potentials change by up to 0.2 V depending on the isomer, and the doublet-quartet energy splitting of compound I, central to “two-state” reactivity, is affected by up to \(-15\) kJ mol\(^{-1}\). These effects are consistently seen with three distinct density functionals, i.e. the effects are not method-dependent. Thus, the nature of the isomer state is an important but overlooked feature of heme chemistry and function, and previous and future studies of hemes may be reconsidered in this new context.

General information
State: Published
Organisations: Department of Chemistry
Authors: Kepp, K. P. (Intern)
Pages: 22355-22362
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Physical Chemistry Chemical Physics
Volume: 19
Issue number: 33
ISSN (Print): 1463-9076
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.06 SJR 1.678 SNIP 1.117
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.771 SNIP 1.244 CiteScore 4.45
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.772 SNIP 1.253 CiteScore 4.29
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.715 SNIP 1.216 CiteScore 4.05
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.916 SNIP 1.184 CiteScore 3.67
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.697 SNIP 1.203 CiteScore 3.6
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.802 SNIP 1.196
Highly Selective Aerobic Oxidation of 5-Hydroxymethyl Furfural into 2,5-Diformylfuran over Mn-Co Binary Oxides

A series of Mn–Co binary oxides were prepared by a simple thermal decomposition procedure and evaluated for the aerobic oxidation of 5-hydroxymethylfurfural (HMF) into 2,5-diformylfuran (DFF). Investigation of the effects of metal amounts and calcination temperatures of the prepared catalysts revealed that the Mn–Co binary oxide with a Mn/Co molar ratio of 1/1 showed the best catalytic performance yielding 42.6% HMF conversion along with 98% selectivity to DFF after 2 h of reaction. The as-prepared catalysts were characterized by nitrogen physisorption, X-ray powder diffraction (XRD), hydrogen temperature-programmed reduction (H2-TPR) and X-ray photoelectron spectroscopy (XPS). These results indicated that the Mn–Co binary oxides could increase the Mn4+/Mn3+ atomic ratio and the exposed lattice oxygen content on the surface, thus accelerating the HMF oxidation into DFF. Furthermore, the Mn–Co binary oxides proved to be reusable in five consecutive reaction runs without significant loss of activity.

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry, Technical University of Denmark, East China University of Science and Technology
Authors: Gui, Z. (Ekstern), Shunmugavel, S. (Intern), Cao, W. (Ekstern), Schill, L. (Intern), Chen, L. (Ekstern), Qi, Z. (Ekstern), Riisager, A. (Intern)
Pages: 6632-6639
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: ChemistrySelect
Volume: 2
Issue number: 23
ISSN (Print): 2365-6549
Ratings:
Web of Science (2018): Indexed yes
Highly Selective Continuous Gas-Phase Methoxycarbonylation of Ethylene with Supported Ionic Liquid Phase (SILP) Catalysts

Supported ionic liquid phase (SILP) technology was applied for the first time to the Pd-catalyzed continuous, gas-phase methoxycarbonylation of ethylene to selectively produce methyl propanoate (MP) in high yields. The influence of catalyst and reaction parameters such as, for example, ionic liquid loading, metal concentration, and ligand loadings was studied, and in particular the SILP catalyst activity and stability was found to be strongly dependent on the ligand to metal ratio.

General information

State: Published
Organisations: Centre for Catalysis and Sustainable Chemistry, Department of Chemistry, Organic Chemistry
Authors: Khokarale, S. G. (Intern), Garcia Suárez, E. J. (Intern), Fehrmann, R. (Intern), Riisager, A. (Intern)
Number of pages: 7
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information

Journal: Chemcatchem
Volume: 9
ISSN (Print): 1867-3880
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
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
Web of Science (2010): Indexed yes
Original language: English
DOIs:
10.1002/cctc.201601428
Source: FindIt
Source-ID: 2357647047
Publication: Research - peer-review › Journal article – Annual report year: 2017
High pressure phase equilibrium of ternary and multicomponent alkane mixtures in the temperature range from (283–473) K

Asymmetric multicomponent alkane mixtures can be used as model systems for reservoir fluids. We have prepared two ternary mixtures, methane/n-butane/n-decane and methane/n-butane/n-dodecane, and two multicomponent mixtures composed of methane/n-butane/n-octane/n-dodecane/n-hexadecane/n-eicosane as model reservoir fluids and measured their phase equilibrium in the temperature range from (283–473) K by using a variable volume cell with full visibility. Their phase envelopes and liquid volume fractions below the saturation pressure have been measured. Four equations of state, including Soave-Redlich-Kwong (SRK), Peng-Robinson (PR), Perturbed Chain Statistical Associating Fluid Theory (PC-SAFT), and Soave-Benedict-Webb-Rubin (Soave-BWR), have been used to predict phase equilibrium of the measured systems. PR and PC-SAFT give better results than others and Soave-BWR gives poor phase envelope predictions which are quite distinct from the predictions by other models. It is generally challenging for any of the tested models to predict all the measured phase envelopes with high accuracy. For predictive calculation of the liquid fractions, the agreement in the low pressure region is good whereas the fractions just below the saturation pressures are difficult to predict. Moreover GERG-2008 has also been tested with the measured methane/n-butane/n-decane system. It over predicts the saturation pressures but predicts low pressure liquid fractions quite accurately.
Ionic liquids have been broadly studied in the past decade for being used as lubricants or lubricant additives. The rheological characterization of these fluids is very important in this context because it determines to a great extent their performance for different lubricants applications, such as hydraulic or gear lubricants. Thus, in this work we have performed the rheometric characterization of two ionic liquids (ILs), 1-ethyl-3-methylimidazolium n-hexylsulfate and trihexyl(tetradecyl)phosphonium tris(pentafluoroethyl)trifluorophosphate, in the temperature range from 298.15 to 353.15 K up to 75 MPa and shear rates up to 1000 s$^{-1}$. For this aim, the setup of a new device for rheological characterization at high pressure based on Couette flow and concentric cylinders was undertaken in this work. Moreover the pressure–viscosity and temperature–viscosity coefficients of these ILs have been calculated. Both ILs present Newtonian behavior in the studied conditions. The trifluorophosphate IL has strong pressure–viscosity dependence, whereas for the other IL this dependence is quite slight.
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.29 SJR 0.88 SNIP 1.097
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.868 SNIP 0.966 CiteScore 1.96
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.021 SNIP 1.208 CiteScore 2.22
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.135 SNIP 1.199 CiteScore 2.17
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.141 SNIP 1.103 CiteScore 2.01
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.862 SNIP 0.988 CiteScore 1.8
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.054 SNIP 1.299
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.313 SNIP 1.037
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.505 SNIP 1.186
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.263 SNIP 1.254
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.146 SNIP 1.33
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.155 SNIP 1.342
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.897 SNIP 1.205
Scopus rating (2003): SJR 1.054 SNIP 1.157
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 0.661 SNIP 1.062
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.978 SNIP 1.234
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 0.735 SNIP 1.16
Scopus rating (1999): SJR 0.891 SNIP 1.249
Original language: English
DOIs:
10.1021/acs.jced.7b00181
High-resolution infrared spectroscopy of CH₂D⁷⁹Br: ro-vibrational analysis of the ν₄ and ν₈ fundamental bands

The high-resolution Fourier transform infrared spectrum of CH₂D⁷⁹Br has been recorded and analysed in the region of the ν₄ and ν₈ fundamentals located in the range 1125–1360 cm⁻¹. The strong ν₄ band, centred at 1225 cm⁻¹, shows an a/b-hybrid structure with predominant a-type character, whereas ν₈, at 1253 cm⁻¹, generates a c-type contour comparable in intensity to the b-type component of ν₄. The upper states of these fundamentals are coupled through a- and b-type Coriolis resonances; further complications in this band system arise from perturbations due to the ν₆ = 2 (1183 cm⁻¹) and ν₅ = ν₆ = 1 (1359 cm⁻¹) dark states. The former interacts with ν₃ = 1 by b-type Coriolis coupling, whereas the latter perturbs the ν₄ = 1 and ν₅ = 1 levels by anharmonic and a-type Coriolis resonances, respectively. Accurate upper state parameters and interaction terms have been determined for the tetrad system ν₄/ν₈/2ν₆/ν₅+ν₆ by also including in the dataset the assigned transitions of the 2ν₆−ν₆ and ν₅+ν₆−ν₆ hot bands obtained from previous analysis.

General information
State: Published
Organisations: Department of Chemistry, Università Ca' Foscari Venezia
Authors: Stoppa, P. (Ekstern), Visinoni, R. (Ekstern), Baldacci, A. (Ekstern), Larsen, R. W. (Intern)
Pages: 1555-1561
Publication date: 2017
Main Research Area: Technical/natural sciences

Publication information
Journal: Molecular Physics
Volume: 115
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ISSN (Print): 0026-8976
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.65 SJR 0.833 SNIP 0.729
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.761 SNIP 0.85 CiteScore 1.68
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.697 SNIP 0.667 CiteScore 1.48
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.678 SNIP 0.715 CiteScore 1.58
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.801 SNIP 0.738 CiteScore 1.62
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.824 SNIP 0.829 CiteScore 1.67
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.786 SNIP 0.722
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.885 SNIP 0.717
BFI (2008): BFI-level 1
Hofmeister Effect on PNIPAM in Bulk and at an Interface: Surface Partitioning of Weakly Hydrated Anions

The effect of sodium fluoride, sodium trichloroacetate, and sodium thiocyanate on the stability and conformation of poly(N-isopropylacrylamide), in bulk solution and at the gold-aqueous interface, is investigated by differential scanning calorimetry, dynamic light scattering, quartz crystal microbalance, and atomic force microscopy. The results indicate a surface partitioning of the weakly hydrated anions, i.e., thiocyanate and trichloroacetate, and the findings are discussed in terms of anion-induced electrostatic stabilization. Although attractive polymer-ion interactions are suggested for thiocyanate and trichloroacetate, a salting-out effect is found for sodium trichloroacetate. This apparent contradiction is explained by a combination of previously suggested mechanisms for the salting-out effect by weakly hydrated anions.
Hydrodeoxygenation of Bio‐polymer Precursors with Base Metal Catalysts

General information
State: Published
Organisations: Centre for Catalysis and Sustainable Chemistry, Department of Chemistry, Organic Chemistry
Authors: Khokarale, S. G. (Intern), Shunmugavel, S. (Intern), Riisager, A. (Intern)
Number of pages: 1
Publication date: 2017

Host publication information
Title of host publication: Book of Abstracts Sustain 2017
Article number: C-6
Main Research Area: Technical/natural sciences
Hydroformylation with Integrated Catalytic-Membrane Separation Reaction System

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry, University of Erlangen-Nuremberg
Authors: Marinkovic, J. M. (Intern), Weiss, A. (Ekstern), Garcia Suárez, E. J. (Intern), Haumann, M. (Ekstern), Riisager, A. (Intern), Fehrmann, R. (Intern)
Number of pages: 1
Publication date: 2017

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Title of host publication: Book of Abstracts Sustain 2017
Article number: C-18
Main Research Area: Technical/natural sciences
Conference: Sustain 2017, Kgs. Lyngby, Denmark, 06/12/2017 - 06/12/2017
Electronic versions:
SustainAbstracts2017c.compressed_33.pdf
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2017

Identification and Quantification of Copper Sites in Zeolites by Electron Paramagnetic Resonance Spectroscopy

Recent quantitative electron paramagnetic resonance spectroscopy (EPR) data on different copper species present in copper exchanged CHA zeolites are presented and put into context with the literature on other copper zeolites. Results presented herein were obtained using ex situ and in situ EPR on copper ion exchanged into a CHA zeolite with Si/Al = 14 ± 1 to obtain Cu/Al = 0.46 ± 0.02. The results shed light on the identity of different copper species present after activation in air. Since the EPR signal is quantifiable, the content of the different EPR active species has been elucidated and Cu2+ in 2Al positions in the 6-membered rings (6mr) of the CHA structure has been characterized. Some copper species are found not to give an EPR signal at ambient or high temperatures. Fortunately, treatments with different gasses under in situ conditions are able to trigger an EPR signal and thus reveal information about the reactivity and the quantity of some of the otherwise EPR silent species. In this way the [Cu–OH]+ species in copper substituted low-Al zeolites has been indirectly observed and quantified. EPR active Cu2+ species have been followed under reduction and oxidation with gas mixtures relevant for the selective catalytic reduction of NO with NH3 (NH3-SCR) revealing that all Cu2+ in 6mr are easily reduced and oxidized at 200 °C. Furthermore, a stable [Cu–NO3]+ species is identified in Cu-CHA after exposure to NO and O2, but is not stable in 2Al 6mr sites of the CHA structure under the applied conditions.

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Department of Chemistry, Organic Chemistry, Haldor Topsoe AS
Authors: Godiksen, A. (Intern), Vennestrøm, P. N. R. (Ekstern), Rasmussen, S. B. (Intern), Mossin, S. (Intern)
In this work, the influence of phosphate buffer and proteins on the potentiometric response of a polymeric membrane-based solid-contact Pb(II) ion-selective electrode (Pb(II)-ISE) was studied. The effects of bovine serum albumin (BSA) adsorption at the surface of the ion-selective membrane combined with electrode conditioning in phosphate-buffered saline (PBS) solution was elucidated by potentiometry and electrochemical impedance spectroscopy. The adsorbed BSA at the surface of the Pb(II)-ISE slightly lowered the detection limit but did not influence the selectivity of the Pb(II)-ISE towards the interfering ions studied (Cu(II), Cd(II)). Conditioning of the Pb(II)-ISE in 0.01 mol dm−3 PBS resulted in a super-Nernstian response which was related to fixation/extraction of Pb(II) in the ion-selective membrane via precipitation of Pb3(PO4)2 by PO4(3-) anions present in PBS. By conditioning of the Pb(II)-ISE in 0.01 mol dm−3 PBS + 1 mg/ml BSA it was possible to extend the linear response range of the Pb(II)-ISE towards lower analyte concentrations. The utilization of this conditioning procedure was validated by determination of Pb(II) concentrations down to ca 20 ppb in aqueous samples by Pb(II)-ISEs and by comparing the results with those obtained by ICP-MS.

**General information**

State: Published
Organisations: Department of Chemistry, NanoChemistry, Organic Chemistry, Abo Akademi University, Malmo University
Authors: Joon, N. K. (Ekstern), He, N. (Ekstern), Wagner, M. (Intern), Cárdenas, M. (Ekstern), Bobacka, J. (Ekstern), Lisak, G. (Ekstern)
Pages: 490-497
Publication date: 2017
Main Research Area: Technical/natural sciences

**Publication information**

Journal: Electrochimica Acta
Volume: 252
ISSN (Print): 0013-4686
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.74 SJR 1.357 SNIP 1.167
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.349 SNIP 1.344 CiteScore 4.86
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.391 SNIP 1.482 CiteScore 4.59
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.435 SNIP 1.607 CiteScore 4.44
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Inorganic ions assisted design and synthesis of all-inorganic halide perovskite nanowires for sustainable solar-energy harvesting

General information
State: Published
Organisations: Department of Chemistry, NanoChemistry, Organic Chemistry
Authors: Tang, Y. (Intern), Chi, Q. (Intern)
Number of pages: 1
Publication date: 2017

Host publication information
Title of host publication: Book of Abstracts, Sustain 2017
Publisher: Technical University of Denmark (DTU)
Article number: M-14
Main Research Area: Technical/natural sciences
Conference: Sustain 2017, Kgs. Lyngby, Denmark, 06/12/2017 - 06/12/2017
Protein amyloid fibrillation is obtaining much focus because it is connected with amyloid-related human diseases such as Alzheimer's disease, diabetes mellitus type 2, or Parkinson's disease. The influence of metal ions on the fibrillation process and whether it is implemented in the amyloid fibrils has been debated for some years. We have therefore investigated the influence and binding geometry of zinc in fibrillated insulin using extended X-ray absorption fine-structure and X-ray absorption near-edge structure spectroscopy. The results were validated with fibre diffraction, Transmission Electron Microscopy and Thioflavin T fluorescence measurements. It is well-known that Zn$^{2+}$ ions coordinate and stabilize the hexameric forms of insulin. However, this study is the first to show that zinc indeed binds to the insulin fibrils. Furthermore, zinc influences the kinetics and the morphology of the fibrils. It also shows that zinc coordinates to histidine residues in an environment, which is similar to the coordination seen in the insulin $R_6$ hexamers, where three histidine residues and a chloride ion is coordinating the zinc.

**General information**

State: Published

Organisations: Department of Chemistry, X-ray Crystallography, Department of Chemical and Biochemical Engineering, The Hempel Foundation Coatings Science and Technology Centre (CoaST), University of Copenhagen, CMCassist Aps

Authors: Frankær, C. G. (Intern), Sønderby, P. (Intern), Bang, M. B. (Intern), Mateiu, R. V. (Intern), Groenning, M. (Ekstern), Bukrinski, J. (Ekstern), Harris, P. (Intern)

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Publication date: 2017

Main Research Area: Technical/natural sciences

**Publication information**

Journal: Journal of Structural Biology

Volume: 199

Issue number: 1

ISSN (Print): 1047-8477

Ratings:

- BFI (2018): BFI-level 1
- Web of Science (2018): Indexed yes
- BFI (2017): BFI-level 1
- Web of Science (2017): Indexed Yes
- BFI (2016): BFI-level 1
- Scopus rating (2016): CiteScore 2.74 SJR 2.664 SNIP 0.905
- BFI (2015): BFI-level 1
- Scopus rating (2015): SJR 3.466 SNIP 1.124 CiteScore 3.12
- Web of Science (2015): Indexed yes
- BFI (2014): BFI-level 1
- Scopus rating (2014): SJR 2.496 SNIP 1.257 CiteScore 3.14
- BFI (2013): BFI-level 1
- Scopus rating (2013): SJR 2.579 SNIP 1.259 CiteScore 3.47
- ISI indexed (2013): ISI indexed yes
- BFI (2012): BFI-level 1
- Scopus rating (2012): SJR 2.254 SNIP 1.231 CiteScore 3.36
- ISI indexed (2012): ISI indexed yes
- BFI (2011): BFI-level 1
- Scopus rating (2011): SJR 2.082 SNIP 1.222 CiteScore 3.47
- ISI indexed (2011): ISI indexed yes
- Web of Science (2011): Indexed yes
- BFI (2010): BFI-level 1
- Scopus rating (2010): SJR 2.586 SNIP 1.187
- BFI (2009): BFI-level 1
- Scopus rating (2009): SJR 2.964 SNIP 1.249
- BFI (2008): BFI-level 1
Interaction between β-lactoglobulin and structurally different heteroexopolysaccharides investigated by solution scattering and analytical ultracentrifugation study

Knowledge on molecular structure of exopolysaccharides (EPSs) and their roles in the associative interactions with proteins is essential to understand the relationship between their structure, physical and rheological properties. Despite their importance, no detailed molecular characterization of bacterial EPSs and their associative interactions with proteins have been reported up to now. By combining X-ray solution scattering (SAXS), dynamic light scattering (DLS) and analytical ultracentrifugation (AUC) in conjunction with scattering modeling, we have characterized four different heteroexopolysaccharides (HePS-1–HePS-4) from lactic acid bacteria (LAB) and their interactions with β-lactoglobulin. We have previously shown that these HePSs exhibited a compact conformation in solution. Here, SAXS data for HePSs (HePS-1–HePS-4) complexes with β-lactoglobulin showed that β-lactoglobulin aggregated strongly with these HePSs. β-lactoglobulin exists as a dimer at pH 4 in the absence of HePSs. When mixed with HePSs, SAXS analysis showed that β-lactoglobulin formed large aggregates. DLS also showed formation of large aggregates of β-lactoglobulin with HePSs, thus validating SAXS data. Turbidity and AUC data indicated that both soluble and insoluble BLG–HePSs complexes were formed. This study provides new insights into the role of molecular structures in associative interactions between HePSs and BLG which has relevance for various industrial applications.

Interlocked graphene-Prussian blue hybrid composites enable multifunctional electrochemical applications

There has been increasing interest recently in mixed-valence inorganic nanostructure functionalized graphene composites, represented by Prussian blue, because they can cost-effectively apply to biosensors and energy devices. In this work, we present a one-pot green method to synthesize interlocked graphene-Prussian Blue hybrid composites as high-performance materials for biosensors and supercapacitor electrodes. Given the fact that graphene oxide (GO) can act as an electron acceptor, we used iron(II) and glucose as co-reducing agents to reduce GO under mild reaction conditions without introducing toxic agents. High quality Prussian blue nanocubes with no or little coordinated water were generated simultaneously. Reduced graphene oxide (rGO) was thus functionalized by Prussian blue nanocubes via chemical bonding to form a kind of interlocked microstructure with high stability and good conductivity. The as-synthesized composites were tested for biosensing of hydrogen peroxide (H2O2) and as supercapacitor electrode materials. The specific capacitance of the microcomposite based electrodes can reach 428 F g⁻¹, with good cycling stability. The microcomposite also displays high performance catalysis towards electroreduction of H2O2 with a high sensitivity of 1.5 A cm⁻² M⁻¹.
Iridoid glucosides in the genus Veronica (Plantaginaceae) from New Zealand

Four simple iridoid glucosides, three known esters of catalpol, seven esters of aucubin, and two phenylethanoids were isolated from Veronica hookeri (syn. Hebe ciliolata; Plantaginaceae). Of these, none of four aromatic (p-methoxybenzoyl, isovanilloyl, veratroyl, caffeoyl) 6-O-esters of aucubin and 6′-O-benzoyl mussaenosic acid, had been reported from nature before. Similarly, three simple iridoid glucosides, two esters of 6-O-rhamnopyranosylcatalpol, and two phenylethanoid glucosides, as well as 1-O-benzoyl-3-a-glucuronosylglycerol, and 1-O-benzoyl rutinoside were isolated from Veronica pinguifolia (syn. Hebe pinguifolia). The compound 3″-O-benzoyl-2″-O-caffeoyl 6-O-rhamnopyranosylcatalpol had not been reported previously. The pattern of the structural features of the iridoid glucosides is overlaid onto the latest molecular phylogenetic framework of Veronica sects. Hebe and Labiatoides, and discussed in the context of evolutionary trends.

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Scopus rating (2013): SJR 1.088 SNIP 1.679 CiteScore 3.63
ISI indexed (2013): ISI indexed yes
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BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.164 SNIP 1.785 CiteScore 3.52
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Scopus rating (2011): SJR 1.024 SNIP 1.642 CiteScore 3.37
Isoform-Specific Substrate Inhibition Mechanism of Human Tryptophan Hydroxylase

Tryptophan hydroxylase (TPH) catalyzes the initial and rate-limiting step in the biosynthesis of serotonin, which is associated with a variety of disorders such as depression and irritable bowel syndrome. TPH exists in two isoforms: TPH1 and TPH2. TPH1 catalyzes the initial step in the synthesis of serotonin in the peripheral tissues, while TPH2 catalyzes this step in the brain. In this study, the steady-state kinetic mechanism for the catalytic domain of human TPH1 has been determined. Varying substrate tryptophan (Trp) and tetrahydrobiopterin (BH$_4$) results in a hybrid Ping Pong-ordered mechanism in which the reaction can either occur through a Ping Pong or a sequential mechanism depending on the concentration of tryptophan. The catalytic domain of TPH1 shares a sequence identity of 81% with TPH2. Despite the high sequence identity, differences in the kinetic parameters of the isoforms have been identified; i.e., only TPH1 displays substrate tryptophan inhibition. This study demonstrates that the difference can be traced to an active site loop which displays different properties in the TPH isoforms. Steady-state kinetic results of the isoforms, and variants with point mutations in a loop lining the active site, show that the kinetic parameters of only TPH1 are significantly changed upon mutations. Mutations in the active site loop of TPH1 result in an increase in the substrate inhibition constant, $K_I$, and therefore turnover rate. Molecular dynamics simulations reveal that this substrate inhibition mechanism occurs through a closure of the cosubstrate, BH$_4$ binding pocket, which is induced by Trp binding.

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Authors: Tidemand, K. D. (Intern), Peters, G. H. (Intern), Harris, P. (Intern), Stensgaard, E. (Ekstern), Christensen, H. E. M. (Intern)
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Karmitoxin: An amine containing polyhydroxy-polyene toxin from the marine dinoflagellate Karlodinium armiger

Marine algae from the genus Karlodinium are known to be involved in fish-killing events worldwide. Here we report for the first time the chemistry and bioactivity of a natural product from the newly described mixotrophic dinoflagellate Karlodinium armiger. Our work describes the isolation and structural characterization of a new polyhydroxy-polyene named karmitoxin. The structure elucidation work was facilitated by use of 13C enrichment and high-field 2D NMR spectroscopy, where
1H–13C long-range correlations turned out to be very informative. Karmitoxin is structurally related to amphidinols and karlotoxins; however it differs by containing the longest carbon–carbon backbone discovered for this class of compounds, as well as a primary amino group. Karmitoxin showed potent nanomolar cytotoxic activity in an RTgill-W1 cell assay as well as rapid immobilization and eventual mortality of the copepod Acartia tonsa, a natural grazer of K. armiger.

**General information**

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Authors: Rasmussen, S. A. (Intern), Binzer, S. B. (Ekstern), Hoeck, C. (Intern), Meier, S. (Intern), Soman De Medeiros, L. (Ekstern), Andersen, N. G. (Intern), Place, A. D. (Ekstern), Nielsen, K. F. (Intern), Hansen, P. J. (Ekstern), Larsen, T. O. (Intern)  
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Scopus rating (2009): SJR 1.461 SNIP 1.5  
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Ligations of Gold Atoms with Iron Porphyrin

Gold is an exotic material with d-electrons deciding electronic mappings and configurations of adsorbed molecules. The specific interaction of Au atoms and S-, N-capped molecules make gold nanoparticles widely applied in the medicine transport and immunoassay. Density functional theory demonstrates that the electronic structure of Au adatoms is $d^9s^1$ but not $d^{10}s^0$ in the forms of Au-thiolates. The surrounding Au surface atoms are passivated leading to both Au-Au and S-S interactions. A wide range of surface phenomena of nanoparticle size-control and break-junctions in surface physics and chemistry including electrochemistry and electrochemical scanning tunneling microscopy (in situ STM) are explained with this theory. Iron porphyrin is a well-known active redox center of cytochrome c and hemoglobin/myoglobin assisting membrane-crossing electron transfer or blood oxygen transport. The electronic states and configurations of iron porphyrin affect the electrochemical properties of the metalloproteins, where the artificial constructed proteins are designed by the mutations of amino residues or the structural optimizations of iron porphyrins. Iron porphyrin adsorption on graphite and graphene surfaces by π-π electron stacking has been widely studied and the catalytic activity found to be enhanced warranting the notion of enzyme mimics. Weak physisorption was, however, recently observed by in situ STM, but the electronic properties of iron porphyrin adsorbed on gold has not been addressed before. This issue is, however, critical. We report here a study of ironporphyrin on the three low-index Au-surfaces using a combination of electrochemistry and density functional theory.

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Long-range interfacial electron transfer and electrocatalysis of molecular scale Prussian Blue nanoparticles linked to Au(111)-electrode surfaces by different chemical contacting groups

We have explored interfacial electrochemical electron transfer (ET) and electrocatalysis of 5–6 nm Prussian Blue nanoparticles (PBNPs) immobilized on Au(111)-electrode surfaces via molecular wiring with variable-length, and differently functionalized thiol-based self-assembled molecular monolayers (SAMs). The SAMs contain positively (~NH$_3^+$) or negatively charged (~COO$^-$) terminal group, as well an electrostatically neutral hydrophobic terminal group (~CH$_3$). The surface microscopic structures of the immobilized PBNPs were characterized by high-resolution atomic force microscopy (AFM) directly in aqueous electrolyte solution under the same conditions as for electrochemical measurements. The
PBNPs displayed fast and reversible interfacial ET on all the surfaces, notably in multi-ET steps as reflected in narrow voltammetric peaks. The ET kinetics can be controlled by adjusting the length of the SAM forming linker molecules. The interfacial ET rate constants were found to depend exponentially on the ET distance for distances longer than a few methylene groups in the chain, with decay factors ($\beta$) of 0.9, 1.1, and 1.3 per CH$_2$, for SAMs terminated by $\text{--NH}_3^+$, $\text{--COO}^-$, and $\text{--CH}_3$, respectively. This feature suggests, first that the interfacial ET processes follow a tunneling mechanism, resembling that of metalloproteins in a similar assembly. Secondly, the electronic contact of the SAM terminal groups that anchor non-covalently the PBNP are crucial as reported for other types of molecular junctions. Highly efficient PBNP electrocatalysis of H$_2$O$_2$ reduction was also observed for the three linker groups, and the electrocatalytic mechanisms analyzed.
Low Temperature DeNOx Technologies for Power and Waste Incineration Plants

Formation of NOx is inevitable during high temperature combustion processes in air. NOx is of increasing environmental concern due to its participation in detrimental photochemical reactions, which lead to ozone layer depletion. NOx emissions also cause acid rain, contributes to smog formation and induces respiratory diseases in humans. There is no doubt that anthropogenic effects are contributing to the global climate change. The largest contributor to anthropogenic greenhouse gas emissions is CO2, been of great interest as a method to decrease global CO2 emissions. Some of the fuels that have drawn particular interest over the past decade is biomass and municipal waste. While the CO2 emissions are decreased by a transition to these fuels, other problems are caused by it. Potassium present in many of the alternative fuels lead to severe deactivation of the catalyst used for NOx abatement. Consequently, NOx abatement is currently not possible when these are used exclusively. Since NOx gasses are strong pollutants, the increased emission caused by using these alternative fuels is highly undesirable and hinders a more widespread use of alternative fuels. The work presented here has primarily been concerned with finding an alternative solution to NOx abatement for biomass and waste incineration. The optimal solution to this would be a tail-end deNOx unit, which operates at low temperatures (60-140°C). Previous work has shown that ionic liquids (ILs) are promising absorbers and can selectively absorb flue gas constituents such as CO2, SO2 and NO. Utilisation of ILs is severely limited by high viscosities, which hinders mass transfer across phase boundary layers. Dispersion of the IL onto a porous support and can selectively absorb flue gas constituents has been investigated. The results S-ILP performed significantly better than any other SILP formulation tested in NO breakthrough experiments. Based on the obtained results, an attempt was made to understand the chemical and physical properties governing the SILP performance. Based on these investigations, characteristics of the optimal support were suggested. It was found that hollow-sphere silica (HS) had properties close to what was considered optimal, therefore it was decided to investigate this support material further. Synthesis of the support material and subsequently SILP formulations utilising the HS-support material were carried out in collaboration with Prof. Dai at Oak Ridge National Laboratory. The resulting HS-SILP performed significantly better than any other SILP formulation tested in NO breakthrough experiments. Based on this performance, it was suggested that the HS-support could be ideal for selective absorption of other gasses using SILP absorbers. Some SILP formulations were found to have significant oxidative capabilities, willingly oxidising NO to higher NOx species. It was found that the observed effect was due to alcohol residuals in the SILP material from the impregnation process, despite careful evaporation and drying. In order to investigate this effect further, the effect of several alcohols were screened and showed promising results. Therefore, an experimental setup was built to investigate if the oxidation would occur under continuous flow conditions, and to determine the steady state oxidation rates. Significant steady state conversions were found under continuous flow conditions, with a high turn over number for methanol. The reaction proceeded over all porous surfaces, but the use of a SILP material seemed to increase the rate of oxidation significantly.

Manganese-Catalyzed Aerobic Heterocoupling of Aryl Grignard Reagents

An improved protocol has been developed for the MnCl2-catalyzed cross-coupling reaction of two arylmagnesium bromides under dioxygen. The reaction was achieved by using the Grignard reagents in a 2:1 ratio and 20 % of MnCl2. Very good yields of the heterocoupling product were obtained when the limiting Grignard reagent underwent little homocoupling under the reaction conditions. Arylmagnesium bromides that contain p-methoxy, p-(dimethylamino), p-fluoro, and p-chloro substituents were shown to afford high product yields in the cross-coupling reactions with a variety of substituted aryl Grignard reagents. Heterocyclic Grignard reagents, on the other hand, were less effective substrates for this transformation because of the rapid homocoupling of these reagents under the reaction conditions.
Manganese-Catalyzed Cross-Coupling of Aryl Halides and Grignard Reagents by a Radical Mechanism

The substrate scope and the mechanism have been investigated for the MnCl₂-catalyzed cross-coupling reaction between aryl halides and Grignard reagents. The transformation proceeds rapidly and in good yield when the aryl halide component is an aryl chloride containing a cyano or an ester group in the para position or a cyano group in the ortho position. A range of other substituents gave no conversion of the aryl halide or led to the formation of side products. A broader scope was observed for the Grignard reagents, where a variety of alkyl- and arylmagnesium chlorides participated in the coupling. Two radical-clock experiments were carried out, and in both cases an intermediate aryl radical was successfully trapped. The cross-coupling reaction is therefore believed to proceed by an SRN1 mechanism, with a triorganomanganate complex serving as the most likely nucleophile and single-electron donor. Other mechanistic scenarios were excluded based on the substrate scope of the aryl halide.
Mechanism of Cobalamin-Mediated Reductive Dehalogenation of Chloroethylenes

Reductive dehalogenation involving cobalamin has been proved to be a promising strategy for decontamination of the polluted environment. However, cob(I)alamin can act both as a strong reductant and a powerful nucleophile, and thus, several competing dehalogenation pathways may be involved. This work uses experimentally calibrated density functional theory on a realistic cobalamin model to resolve controversies of cobalamin-mediated reduction of chloroethylenes by exploring mechanisms of electron transfer, nucleophilic substitution, and nucleophilic addition. The computational results provide molecular-level insight into the competing pathways for chloroethylenes reacting with cob(I)alamin: the computed ratios of inner-sphere to outer-sphere pathways for perchloroethylene and trichloroethylene are 17:1 and 3.5:1, respectively, in accord with the corresponding experimental ratios of >10:1 and >2.3:1, while the computed outer-sphere pathway for other less-chlorinated ethylenes is hampered by high barriers (>25 kcal/mol). Thus, a new mechanistic picture has been obtained in which the highly chlorinated ethylenes primarily react via an inner-sphere nucleophilic-substitution pathway, whereas the less-chlorinated ethylenes mainly react through an inner-sphere nucleophilic-addition pathway. Especially, the quantitative comparison of standard reduction potentials between the formed chlorinated-cobalamin and cob(I)alamin/cob(I)alamin couple can be used to distinguish whether the inner-sphere pathway can proceed or not, and linear free-energy relationships have been developed to predict the reductive dehalogenation reactivity within a given mechanism. Finally, we propose new dual-isotope analyses for distinguishing the various environmental dehalogenation mechanisms.

General information
Membrane dynamics of γ-secretase provides a molecular basis for Aβ binding and processing

γ-secretase produces β-amyloid (Aβ) within its presenilin (PS1) subunit, mutations in which cause Alzheimer’s disease, and current therapies thus seek to modulate its activity. While the general structure is known from recent electron microscopy studies, direct loop- and membrane-interactions and explicit dynamics relevant to substrate processing remain unknown. We report a modeled structure utilizing the optimal multi-template information available, including loops and missing side chains, account of maturation cleavage, and explicit all-atom molecular dynamics in the membrane. We observe three distinct conformations of γ-secretase (open, semi-open, and closed) that remarkably differ by tilting of helix 2 and 3 of PS1, directly controlling active site availability. The large hydrophilic loop of PS1 where maturation occurs reveals a new helix segment that parallels the likely helix character of other substrates. The semi-open conformation consistently shows the best fit of Aβ peptides, i.e. longer residence before release and by inference more trimming. In contrast, the closed, hydrophobic conformation is largely inactive and the open conformation is active but provides fewer optimal interactions and induces shorter residence time and by inference releases Aβ peptides of longer lengths. Our simulations thus provide a molecular basis for substrate processing and changes in the Aβ42/Aβ40 ratio. Accordingly, selective binding to protect the semi-open “innocent” conformation provides a molecular recipe for effective γ-secretase modulators; we provide the full atomic structures for these states that may play a key role in developing selective γ-secretase modulators for treatment of Alzheimer’s disease.
Metal-Organic Framework Derived FeP/C Interlocked Graphene Hybrid Composite for Hydrogen Evolution Reaction

We report the design and nanoengineering of carbon-film-coated iron sulfide nanorods (C@Fe$_7$S$_8$) as an advanced conversion-type lithium-ion storage material. The structural advantages of the iron-based metal-organic framework (MIL-88-Fe) as both a sacrificed template and a precursor are explored to prepare carbon-encapsulated poly iron sulfide through solid-state chemical sulfurizing. The resulting core-shell nanorods consisting of approximately 13% carbon and 87% Fe$_7$S$_8$ have a hierarchically porous structure and a very high specific surface area of 277 m$^2$g$^{-1}$. When tested for use in fabrication of a redox conversion-type lithium-ion battery, this composite material has demonstrated high lithium-ion storage capacity at 1148 mA h g$^{-1}$ under the current rate of 500 mA g$^{-1}$ for 170 cycles and an impressive rate-retention...
capability at 657 mA h g\(^{-1}\) with a current density of 2000 mA g\(^{-1}\). On the basis of systematic structural analysis and microscopic mapping, we discuss the charge-discharge mechanisms and the crucial factors associated with the stability and structural changes upon charge-discharge cycling.

**Microfabricated Nanofluidic cells for in situ liquid TEM**

Over the last decade, transmission electron microscopy (TEM) has been revolutionized not only by the introduction of new and very sophisticated hardware for improved resolution, such as aberration correctors and monochromators, but also by the improvement of new methods that have provided more than structural information of materials. In this regard, in situ liquid cell electron microscopy (EM) is one of the new emerging methods that gained a lot of attention by making possible to observe processes and samples in liquid environments within the chamber of an electron microscope.

The main focus of this PhD project is to improve the technologies behind liquid cell TEM by developing a novel and robust liquid cell device able to increase the control over the liquid layer thickness, essential for good imaging conditions. A new type of nanofluidic cell has been created with an architecture based on wafer bonding of Atomic layer deposited (ALD) Al\(_2\)O\(_3\) on Si\(_3\)N\(_4\) membranes. With the improved liquid layer thickness control, we use the devices to measure the electron mean free path in water which is a fundamental aspect of TEM studies, and present the high-resolution TEM capabilities of the nanofluidic cell. Furthermore, the first findings on nanoparticle (NP) growth in this particular nanochannel system are presented that also opens up for new types of liquid cell studies with laminar flow. These results demonstrate the capability of the novel nanofluidic cell to provide ultra-thin liquid layers, allowing quantitative and high-precision acquisition of liquid thickness maps, high resolution observations and meaningful information about synthesis of NPs from metal precursor solutions in confined space.

Finally, a new concept device based on a Si\(_3\)N\(_4\) membrane for plunge freezing fixation, which enables ultra-fast cooling rates, is presented.
Modeling of Shale Gas Adsorption and its Influence on Phase Equilibrium

Natural gas and oil produced from shale accounts for a significant portion in the global production. Due to the large surface area and high organic content in shale formations, adsorption plays a major role in the storage of the hydrocarbons within the rock and their phase equilibrium. This study provides a comparison of several engineering models for gas adsorption in shale based on the recent literature data for pure and binary gases. For pure components, Langmuir, the modified Toth-Langmuir, and the Multicomponent Potential Theory of Adsorption using Dubinin-Radushkevich potential (MPTA-DRA) were compared. The three models show similar deviations lower than 10%. For binary gases, Multicomponent Langmuir (ML), Ideal Adsorbed Solution Theory (IAST) and MPTA were evaluated, where MPTA shows the lowest deviation with 17.9%. Additionally, we presented an analysis of the phase envelope shift under the influence of the capillary pressure and the adsorption film. ML and IAST were used to calculate the adsorption amount whereas MPTA was used to generate artificial adsorption data over large temperature range and for other homologous hydrocarbons to estimate the ML and IAST parameters. The adsorption film thickness was considered in the calculation of the effective capillary radius and the corresponding capillary pressure. The combined effects modify the saturation pressure in the whole temperature range except at the critical point. The biggest impact was found on the bubble point branch away from the critical point where the interfacial tension of the system is more pronounced.

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Modeling Study of High Pressure and High Temperature Reservoir Fluids

With dwindling easily accessible oil and gas resources, more and more exploration and production activities in the oil industry are driven to technically challenging environments such as unconventional resources and deeper formations. The temperature and pressure can become extremely high, e.g., up to 250 °C and 2400 bar, in the deep petroleum reservoirs. Furthermore, many of these deep reservoirs are found offshore, including the North Sea and the Gulf of Mexico, making the development even more risky. On the other hand, development of these high pressure high temperature (HPHT) fields can be highly rewarding if successfully produced. This PhD project is part of the NextOil (New Extreme Oil and Gas in the Danish North Sea) project which is intended to reduce the uncertainties in HPHT field development. The main focus of this PhD is on accurate description of the reservoir fluid behavior under HPHT conditions to minimize the production risks from these types of reservoirs. In particular, the study has thoroughly evaluated several non-cubic Equations of State (EoSs) which are considered promising for HPHT fluid modeling, showing their advantages and short comings based on an extensive comparison with experimental data. In the course of the evaluation, we have developed new petroleum fluid characterization procedures, built large databases for well-defined mixtures and reservoir fluids, and improved the evaluation software and made it more suitable for efficient and large scale comparison. We have made a comprehensive comparison between cubic and non-cubic EoSs to evaluate whether advanced EoS in non-cubic forms, including both the SAFT-type EoS with strong theoretical basis (e.g. the PC-SAFT EoS) and the empirical BWR-type EoS (e.g. the Soave-BWR EoS), can be advantageous for describing the physical properties and phase equilibrium of reservoir fluids over a wide temperature and pressure range. In addition, we have also compared these models in calculation of heat capacities and Joule-Thomson coefficients for pure components and multicomponent mixtures. Joule-Thomson coefficients are of special interest to the oil industry because of the so called reverse Joule-Thomson effect commonly observed in HPHT
fields, where a decrease in pressure results in an increase in temperature, which is just the opposite to the effect at low pressure. In the comparative studies between cubic and non-cubic models, we also included GERG-2008 which is a wide-range EoS developed for 21 components of natural gases and their binary mixtures and is regarded as the most accurate EoS model for natural gas mixtures. It was found that the non-cubic models are much better than the cubics in density, compressibility, heat capacity and Joule-Thomson coefficient calculation of the well defined light and heavy components in reservoir fluids over a wide temperature and pressure range, GERG-2008 being the best with the lowest deviation among all EoS models. GERG-2008 however gives very large deviations for bubble point pressure calculation of some heavy and asymmetric binary systems such as n-butane + n-nonane system. This suggests that this EoS and its binary interaction parameters could still be improved for some of the binary pairs. Soave-BWR gives the closest prediction of the thermal properties to that of GERG-2008 among other EoSs tested in this study. The binary VLE calculation showed that PC-SAFT and Soave-BWR are similar to SRK and PR in correlating the important binary pairs in reservoir fluids. Although Soave-BWR and PC-SAFT give smaller average kij values than SRK and PR, they are more sensitive to the change in kij. Phase envelope prediction of synthetic gases showed that all the EoS models were similar for not too asymmetric synthetic gases, with or without the optimal kij values for SRK, PR, PC-SAFT and Soave-BWR. For highly asymmetric synthetic mixtures, Soave-BWR and GERG-2008 tend to predict phase envelopes different from other models where as none of the tested models give satisfactory predictions. For heat capacity and Joule-Thomson coefficients, GERG-2008 and Soave-BWR give the closest predictions. All the evaluated EoS models tend to predict a nearly constant Joule-Thomson coefficient at high pressures. For typical reservoir temperatures, the constant is around -0.5 K/MPa. For non-cubic models like PC-SAFT the characterization method is less mature than the cubic models. A reservoir fluid characterization method for PC-SAFT has been proposed by combining Pedersen’s method with a newly developed set of correlations for the PC-SAFT model parameters m, mε/k and mσ. In addition, we further improved the characterization method for PC-SAFT by adjusting the correlations with a large PVT database. We have further improved the correlations and more importantly, we have established a general approach to characterizing reservoir fluids for any EoS. The approach consists in developing correlations of model parameters first with a database for well-defined components and then adjusting the correlations with a large PVT database. The adjustment is made to minimize the deviation in key PVT properties like saturation pressures, densities at reservoir temperature and Stock Tank Oil (STO) densities, while keeping the n-alkane limit of the correlations unchanged. Apart from applying this general approach to PC-SAFT, we have also shown that the approach can be applied to classical cubic models like SRK and PR. In addition, we discussed how to develop a PNA based characterization for PC-SAFT and also utilize a large PVT database to further improve the characterization. With the developed characterization methods, we have made a comparison in PVT calculation involving 17 EoS-characterization combinations and 260 reservoir fluids. PC-SAFT with the new general characterization method is shown to give the lowest AAD% and maximum deviation in calculation of saturation pressure, density and STO density, among all the tested characterization methods for PC-SAFT. Application of the new characterization method to SRK and PR improved the saturation pressure calculation in comparison to the original characterization method for SRK and PR. Using volume translation together with the new characterization approach for SRK and PR gives comparable results for density and STO density to that of original characterization for SRK and PR with volume translation. For the PVT database used in this study, cubic EoSs seem to have better performance than PC-SAFT in calculation of saturation pressure; PC-SAFT and cubics with volume translation show comparable results in calculation of density and STO density. As a preliminary attempt to integrate more analytical information in characterization, we discussed how to modify the existing algorithms to utilize data from both simulated distillation and true boiling point distillation, and in particular, the component distribution information from the simulated distillation. Some analyses have been made on the impact of including more detailed analytical information. Finally, to improve Soave-BWR for mixture calculation, we have tried to develop several new sets of mixing rules for this EoS. The new mixing rules were developed based on some theoretical considerations as well as the previous mixing rules for non-cubic EoS models. In addition, it was tried to create some hybrid mixing rules by combining a new set of mixing rules and the original mixing rules for Soave-BWR. It was shown that some problems with the original Soave-BWR mixing rules can be fixed by the new mixing rules although the overall performance is not significantly improved. Development of mixing rules for non-cubic EoS models is still a semi-empirical process, requiring extensive testing to evaluate their performance. We have developed the code in a structured manner so that the new mixing rules can be quickly tested. It can facilitate further extensive screening of new mixing rules for Soave-BWR or even other non-cubic EoS models.

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Organisations: Department of Chemistry, Center for Energy Resourses Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Ressources Engineering
Authors: Varzandeh, F. (Intern), Yan, W. (Intern), Stenby, E. H. (Intern)
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Modifications of TIGIT expression contribute to CD8 T cell exhaustion in chronic virus infection

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Organisations: Department of Chemistry, Department of Systems Biology, Center for Biological Sequence Analysis, Department of Bio and Health Informatics, Genomic Epidemiology, Karolinska Institutet, University of Pennsylvania, National Institute of Respiratory Diseases, University of California, San Francisco
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BFI (2012): BFI-level 1
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ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.854 SNIP 0.66 CiteScore 2.06
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.844 SNIP 0.622
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.962 SNIP 0.662
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Molecular Switching in Confined Spaces: Effects of Encapsulating the DHA/VHF Photo-Switch in Cucurbiturils

Confinement of reactive chemical species uniquely affects chemical reactivity by restricting the physical space available and by restricting access to interactions with the solvent. In Nature, for example, confined protein binding pockets govern processes following photoisomerization reactions and the isomerizations themselves. Here we describe the first example of a dihydroazulene/vinylheptafulvene (DHA/VHF) photo-switch functioning in water, and we show how its switching behavior is strongly influenced by supramolecular interactions with a series of cucurbit[n]uril (CB) host molecules. In CB7 inclusion complexes, the kinetics of the thermal VHF-to-DHA back-reaction is accelerated, while in CB8 inclusion complexes, the kinetics is slowed down as compared to the free photo-switch. The effect of the CB encapsulation of the photo-switch can be effectively canceled by introducing a guest that binds the CB more strongly. According to DFT calculations, a stabilization of the reactive s-cis VHF conformer relative to the s-trans VHF appears to be a contributing factor responsible for the accelerated back-reaction when encapsulated in CB7.

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Organisations: Department of Chemistry, Organic Chemistry, University of Copenhagen
Authors: Petersen, M. Å. (Ekstern), Rasmussen, B. (Ekstern), Andersen, N. N. (Ekstern), Sauer, S. P. (Ekstern), Nielsen, M. B. (Ekstern), Beeren, S. R. (Intern), Pittelkow, M. (Ekstern)
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Nanoengineering of graphene supported functional composites for performance enhanced enzymatic biofuel cells

General information
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Organisations: Department of Chemistry, NanoChemistry, Organic Chemistry
Authors: Shen, F. (Intern), Cao, X. (Intern), Pankratov, D. (Intern), Zhang, J. (Intern), Chi, Q. (Intern)
Pages: 219-240
Nano-glass ceramic cathodes for Li+/Na+ mixed-ion batteries

Electrode materials can display superior electrochemical performances and behavior via the nanoscale design. Here, the low-temperature synthesis of nano-glass ceramics (NGCs) is based on inheriting the network structure of yeast polyphosphate metabolism. The NGCs-3 sample synthesized with a molar ratio of Fe/V = 7:6 is composed of nanodomains of semiconducting oxide glass (Li2O-Na2O-Fe2O3-V2O5-P2O5, LNFVP), nanocrystalline particles (Li9Fe3P8O29, Li0.6V1.67O3.67 and VOPO4), and nanopores connected by interfaces. We have clarified the mixing ion transport mechanism and the electrochemical reactions, and the influences of molar ratio of Fe/V on the structure and electrochemical properties of NGCs. This nanoscale design offers a new possibility improved the electrochemical performances of Li+/Na+ mixed-ion batteries (LNMIBs). The NGCs-3 electrode exhibits a higher discharge capacity (145 mAh g$^{-1}$) and energy storage density (525 Wh kg$^{-1}$) at 5C, and the capacity retention reaches 70% after 1000 cycles. More importantly, we have established a direct relationship between the electrochemical kinetics and nanostructure of NGC electrode materials.
ISI indexed (2012): ISI indexed yes
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ISI indexed (2011): ISI indexed yes
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Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 2.117 SNIP 1.793
Web of Science (2009): Indexed yes
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Scopus rating (2008): SJR 1.968 SNIP 1.726
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.597 SNIP 1.489
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.8 SNIP 2.224
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.65 SNIP 1.825
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Scopus rating (2003): SJR 1.66 SNIP 1.583
Scopus rating (2002): SJR 1.959 SNIP 1.4
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Nanoscale engineering of 3D graphene foams for enzyme immobilization and enhanced bioelectrocatalysis

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Organisations: Department of Chemistry, NanoChemistry, Organic Chemistry, Novozymes A/S
Authors: Shen, F. (Intern), Zhang, J. (Intern), Ulstrup, J. (Intern), Østergaard, L. H. (Ekstern), Chi, Q. (Intern)
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New class of two-dimensional bimetallic nanoplatelets for high energy density and electrochemically stable hybrid supercapacitors
Currently, the application of supercapacitors (SCs) in portable electronic devices and vehicles is limited by their low energy density. Developing high-energy density SCs without sacrificing their advantages, such as their long-term stability and high power density, has thus become an increasing demand but a major challenge. This demand has motivated tremendous efforts, especially towards discovering and optimizing the architecture of novel electrode materials. To this end, we herein report the design, synthesis, and SC application of a new family of two-dimensional (2D) nanoplatelets, i.e., a transition-metal hydroxymethylate complex (Ni_{x}Co_{1-x}(OH)(OCH_{3})). Bimetallic nanoplatelets were synthesized via a cost-effective approach involving a one-step solvothermal procedure. We for the first time tuned the metal composition of these 2D nanoplatelets over the entire molar-fraction range (0 - 1.0). Tuning the molar ratio of Ni/Co allowed us to optimize the structures and physicochemical properties of the nanoplatelets for SC applications. When tested in a half cell, SC electrodes using the nanoplatelets exhibited high electrochemical performance with a specific capacitance as high as 1,415 F⋅g^{-1} and a 96.1% retention of the initial capacitance over 5,000 cycles. We exploited the novel 2D nanoplatelets as cathode materials to assemble a hybrid SC for full-cell tests. The resulting SCs operated in a wide potential window of 0 - 1.7 V, exhibited a high energy density over 50 Wh⋅kg^{-1}, and sustained their performance over 10,000 charge-discharge cycles. The results suggest that the novel 2D nanoplatelets are promising alternative materials for the development of high-energy density SCs.
New degradation compounds from lignocellulosic biomass pretreatment: routes for formation of potent oligophenolic enzyme inhibitors

In this study 26 new oligophenol cellulase inhibitors were discovered from wheat straw pretreatment liquors. By consideration of the reaction mechanisms for their formation it is proposed that these oligophenols are formed during hydrothermal biomass pretreatment by pentose self-condensation reactions involving aldol condensations, 1,4 additions to α,β unsaturated carbonyl compounds, 3-keto acid decarboxylations and oxidations. Furthermore, pentose reactions with phenolic lignin components are suggested. The identification of the central role of xylose in the reaction routes for oligophenolic inhibitor formation led to the solution to protect the reactive anomeric center in xylose. It is shown that protection of the anomeric center in in situ generated xylose with ethylene glycol monobutyl ether, during pretreatment of wheat straw, reduces the level of oligophenols by 73%. The results pave the way for implementation of new types of reactions that hinder inhibitor formation in lignocellulosic biomass processing.

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Organisations: Department of Chemistry, Organic Chemistry, Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, DONG Energy AS, DONG Energy A/S
Authors: Rasmussen, H. (Ekstern), Tanner, D. A. (Intern), Sørensen, H. R. (Ekstern), Meyer, A. S. (Intern)
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Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.398 SNIP 2.007 CiteScore 8.05
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Scopus rating (2013): SJR 2.266 SNIP 1.815 CiteScore 7.44
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Scopus rating (2012): SJR 2.439 SNIP 1.709 CiteScore 6.64
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ISI indexed (2011): ISI indexed yes
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BFI (2010): BFI-level 2
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New electrochemiluminescence catalyst: Cu2O semiconductor crystal and the enhanced activity of octahedra synthesized by iodide ions coordination

Cuprous oxide (Cu2O) crystals are usually used as the photocatalysts of water splittings and carbon monoxide oxidations. Herein, we report the new catalytic properties of Cu2O to the electrochemiluminescence (ECL) reactions of luminol and oxygen. Adjusting the shape of Cu2O microcrystals from cube to octahedra also facilitates the improved electrocatalytic activity, where octahedral Cu2O microcrystals possess higher ECL signal by 25% at -0.6 V (versus Ag/AgCl) at pH 7.4. The octahedral Cu2O microcrystals are synthesized by the coordination of iodide ions to the surface, which alters the crystals shapes from cubes to octahedra. Size-distribution of octahedra is improved with this method compared to the previous studies with only hydroxide ions as the coordinates. The catalytic activity of octahedral Cu2O crystals is expected to be compared with the noble metal nanomaterials and constructed the high-efficiency and low-cost ECL biosensors.
New Fluorescent Nanoparticles for Ultrasensitive Detection of Nucleic Acids by Optical Methods
For decades the detection of nucleic acids and their interactions at low abundances has been a challenging task that has thus far been solved by enzymatic target amplification. In this work we aimed at developing efficient tools for amplification-free nucleic acid detection, which resulted in the synthesis of new fluorescent nanoparticles. Here, the fluorescent nanoparticles were made by simple and inexpensive radical emulsion polymerization of butyl acrylate in the presence of fluorescent dyes and additional functionalization reagents. This provided ultra-bright macrofluorophores of 9-84nm mean diameter, modified with additional alkyne and amino groups for bioconjugation. By using click and NHS chemistries, the new nanoparticles were attached to target-specific DNA probes that were used in fluorimetry and fluorescence microscopy. Overall, these fluorescent nanoparticles and their oligonucleotide derivatives have higher photostability, brighter fluorescence and hence dramatically lower limits of target detection than the individual organic dyes. These properties make them useful in approaches directed towards ultrasensitive detection of nucleic acids, in particular for imaging and in vitro diagnostics of DNA.

General information
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Scopus rating (2016): CiteScore 2.64 SJR 1.242 SNIP 0.733
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Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.386 SNIP 0.852 CiteScore 2.88
Web of Science (2014): Indexed yes
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Scopus rating (2013): SJR 1.622 SNIP 0.849 CiteScore 3.15
ISI indexed (2013): ISI indexed yes
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BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.853 SNIP 0.902 CiteScore 3.49
ISI indexed (2012): ISI indexed yes
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BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.903 SNIP 0.952 CiteScore 3.59
ISI indexed (2011): ISI indexed yes
New Motifs in Deoxydehydration: Beyond the Realms of Rhenium

The deoxydehydration (DODH) reaction remains one of the most efficient methods of reducing the oxygen content of biomass while keeping important functionality in place. This reaction is traditionally catalysed by high-valent oxo-rhenium species. Recent research into heterogeneous rhenium-based catalysts for DODH demonstrates their ability to rival and in some cases surpass their homogeneous counterparts. Furthermore, catalysts based on the metals molybdenum and vanadium show great potential as inexpensive alternatives to rhenium catalysts. In this Minireview, we detail the recent developments within the field of DODH with particular emphasis on discoveries outside the realms of rhenium.

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Organisations: Department of Chemistry, Organic Chemistry
Authors: Petersen, A. R. (Intern), Fristrup, P. (Intern)
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Scopus rating (2015): SJR 2.416 SNIP 1.184 CiteScore 4.99
New pentose dimers with bicyclic moieties from pretreated biomass

In lignocellulosic biorefinery processes involving enzyme catalysed reactions it is a challenge that enzyme inhibiting compounds are generated and liberated during pretreatment of the biomass. In this study the contribution to cellulase inhibition from xylooligosaccharides and newly discovered oligophenolic compounds from pilot scale pretreated wheat straw was assessed at two different pretreatment severities. An increase in severity of the pretreatment led to more oligophenol compounds and in turn the total overall cellulase inhibition increased. When the xylooligosaccharides were enzymatically degraded prior to cellulose hydrolysis, a relief in cellulase inhibition was observed, but some inhibition...
remained, suggesting that other components also played a role in inhibition. We propose that these components include dipentoses with bicyclic moieties and feruloylated tripentoses, because LC-MS/MS analysis revealed the presence of these components in the liquid from hydrothermal pretreated wheat straw after enzymatic treatment. The reaction mechanisms for synthesis of the new dipentoses having hydroxylated oxane bicyclic residues are considered and they are proposed to be formed as reaction products from either xylose or glucose reacting with glyceraldehyde during pretreatment. The data show that the main cellulase inhibition from hydrothermally pretreated wheat straw liquors is due to xylooligosaccharides followed by oligophenolic compounds and the newly discovered dipentose with bicyclic moieties and feruloylated tripentoses. The relative amounts and hence contribution to inhibition from each class of compounds changes with severity of the pretreatment.

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Organisations: Department of Chemistry, Organic Chemistry, Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, DONG Energy A/S
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Scopus rating (2016): CiteScore 3.06 SJR 0.875 SNIP 0.743
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BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.959 SNIP 0.837 CiteScore 3.42
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.114 SNIP 0.965 CiteScore 3.87
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.117 SNIP 0.903 CiteScore 3.74
ISI indexed (2013): ISI indexed yes
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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**

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Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry, Center for Electron Nanoscopy
Authors: Kramer, S. (Intern), Mielby, J. J. (Intern), Buss, K. S. (Intern), Kasama, T. (Intern), Kegnæs, S. (Intern)
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- 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
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- Scopus rating (2013): SJR 2.167 SNIP 1.06 CiteScore 4.82
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- Scopus rating (2012): SJR 2.375 SNIP 1.142 CiteScore 4.58
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- Scopus rating (2011): SJR 2.238 SNIP 1.056 CiteScore 4.3
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**NMR Isotope Tracking Reveals Cascade Steps in Carbohydrate Conversion by Sn-Beta**

Quantitative isotope tracking studies were used to investigate the reaction pathways occurring for Sn-Beta catalyzed carbohydrate conversion to various alpha-hydroxy esters. Experimental insight into the conversion of pentoses was sought (i) by identifying pathways based on isotope patterns in the reaction products and (ii) through probing asymmetric isotope incorporation into products. The results indicate that reaction intermediates remain coordinated to the active site.
throughout the reaction cascades, regardless of the reaction pathway. A predominant transformation of the C1 carbohydrate position to the C3 position of methyl lactate resembles enzymatic glycolysis. Likewise, the majority of retro-aldol cleavage occurs from the carbohydrate in the ketose form, again resembling biological glycolysis. In addition, various side-activities are detected in Sn-Beta catalyzed carbohydrate conversion, including 5,1-hydride and 1,2-carbon shift reaction of the carbohydrates.

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Organisations: Department of Chemistry, Organic Chemistry, Haldor Topsoe AS
Authors: Elliot, S. G. (Intern), Taarning, E. (Ekstern), Madsen, R. (Intern), Meier, S. (Intern)
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Scopus rating (2014): SJR 1.88 SNIP 1.102 CiteScore 4.52
Web of Science (2014): Indexed yes
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Scopus rating (2013): SJR 2.167 SNIP 1.06 CiteScore 4.82
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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
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**Off-Pathway Intermediates in the Conversion of Sugars to Plastic**

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Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry, Haldor Topsoe AS
Authors: Tosi, I. (Intern), Riisager, A. (Intern), Taarning, E. (Ekstern), Meier, S. (Intern)
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**Host publication information**
Title of host publication: Book of Abstracts Sustain 2017
On the elusive crystal structure of expanded austenite

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

We have used high-resolution quasielastic neutron scattering (QENS) to investigate the dynamics of water molecules (time scale of motion similar to ~10^-11 - 10^-9 s) in proximity to single-supported bilayers of the zwitterionic lipid DMPC (1,2-dimyristoyl-sn-glycero-3-phosphorylcholine) and the anionic lipid DMPG (1,2-dimyristoyl-sn-glycero-3-phosphoglycerol) in the temperature range 160-295 K. For both membranes, the temperature dependence of the intensity of neutrons scattered elastically and incoherently from these samples indicates a series of freezing/melting transitions of the membrane-associated water, which have not been observed in previous studies of multilayer membranes. We interpret these successive phase transitions as evidence of different types of water that are common to the two membranes and which are defined by their local environment: bulk-like water located furthest from the membrane and two types of confined water in closer proximity to the lipids. Specifically, we propose a water type termed "confined 2" located within and just above the lipid head groups of the membrane and confined 1 water that lies between the bulk-like and confined 2 water. Confined 1 water is only present at temperatures below the freezing point of bulk-like water. We then go on to determine the temperature dependence of the translational diffusion coefficient of the water associated with single-supported DMPG membranes containing two different amounts of water as we have previously done for DMPC. To our knowledge, there have been no previous studies comparing the dynamics of water in proximity to zwitterionic and anionic membranes. Our analysis of the water dynamics of the DMPG and DMPC membranes supports the classification of water types that we have inferred from their freezing/melting behavior. However, just as we observe large differences in the freezing/melting behavior between these model membranes for the samewater type, our measurements demonstrate variation between these membranes in the dynamics of their associated water over a wide temperature range. In particular, there are differences in the diffusive motion of water closest to the lipid head groups. Previously, QENS spectra of the DMPC membranes have revealed the motion of water bound to the lipid head groups. For the DMPG membrane, we have found some evidence of such bound water molecules; but the signal is too weak for a quantitative analysis. However, we observe confined 2 water in the DMPG membrane to undergo slow translational diffusion in the head group region, which was unobserved for DMPC. The weak temperature dependence of its translational diffusion coefficient allows extrapolation to physiological temperatures for comparison with molecular dynamics simulations.

General information
Optical absorption and magnetic circular dichroism spectra of thiouracils: a quantum mechanical study in solution

The excited electronic states of 2-thiouracil, 4-thiouracil and 2,4-dithiouracil, the analogues of uracil where the carbonyl oxygens are substituted by sulphur atoms, have been investigated by computing the magnetic circular dichroism (MCD) and one-photon absorption (OPA) spectra at the time-dependent density functional theory level. Special attention has been paid to solvent effects, included by a mixed discrete/continuum model, and to determining how our results depend on the adopted DFT functional (CAM-B3LYP and B3LYP). Whereas including solvent effects does not dramatically impact the MCD and OPA spectra, though improving the agreement with the experimental spectra, the performances of CAM-B3LYP and B3LYP are remarkably different. CAM-B3LYP captures well the effect of thionation on the uracil excited states and provides spectra in good agreement with the experiments, whereas B3LYP shows some deficiency in describing 2-TU and 2,4-DTU spectra, despite being more accurate than CAM-B3LYP for 4-TU.

General information
State: Published
Organisations: Department of Chemistry, Consiglio Nazionale delle Ricerche, KTH - Royal Institute of Technology
Authors: Martínez-Fernández, L. (Ekstern), Fahleson, T. (Ekstern), Norman, P. (Ekstern), Santoro, F. (Ekstern), Coriani, S. (Intern), Improta, R. (Ekstern)
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BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.37 SJR 0.722 SNIP 0.799
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.805 SNIP 0.811 CiteScore 2.4
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.874 SNIP 0.946 CiteScore 2.55
Web of Science (2014): Indexed yes
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Scopus rating (2013): SJR 0.989 SNIP 1.006 CiteScore 3
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Heavy 5d elements, like osmium, feature strong spin-orbit interactions which are at the origin of exotic physical behaviors. Revealing the full potential of, for example, novel osmium oxide materials ("osmates") is however contingent upon a detailed understanding of the local single-ion properties. Herein, two molecular osmate analogues, [OsF$_6$]$_2^-$ and [OsF$_6$]$^-$, are reported as model systems for Os$^{4+}$ and Os$^{5+}$ centers found in oxides. Using X-ray absorption spectroscopy (XAS) and X-ray magnetic circular dichroism (XMCD) techniques, combined with state-of-the-art ab initio calculations, their ground state was elucidated; mirroring the osmium electronic structure in osmates. The realization of such molecular model systems provides a unique chemical playground to engineer materials exhibiting spin-orbit entangled phenomena.
Phase Equilibrium Modeling for Shale Production Simulation

Production of oil and gas from shale reservoirs has gained more attention in the past few decades due to its increasing economic feasibility and the size of potential sources around the world. Shale reservoirs are characterized by a more tight nature in comparison with conventional reservoirs, having pore size distributions ranging in the nanometer scale. Such a confined nature introduces new challenges in the fluid phase behavior. High capillary forces can be experienced between
the liquid and vapor, and selective adsorption of components onto the rock becomes relevant. The impact of these effects is of great importance to understanding the storage of hydrocarbons inside and to forecasting its production. In this thesis, a study focused on the effects of capillary pressure and adsorption on phase behavior, and their impact on oil production is provided. An efficient algorithm for phase envelope calculations in the presence of the capillary pressure is presented, and it is used to analyze the main changes on the phase boundary for several fluids of interest. The results show changes in the saturation pressure and temperature along the phase envelope, except at the critical point. A linear analysis is presented to explain such changes, as a result, useful mathematical relationships that estimate the magnitude of these changes were obtained. Moreover, a flash algorithm that accounts for capillarity was developed. The algorithm was implemented into a fully implicit compositional reservoir simulator, which was then used to assess the impact of the capillary pressure on phase behavior in oil and gas production from tight reservoirs. Since capillary pressure and adsorption occur simultaneously in shale, its combined effect was studied. A model comparison for high-pressure adsorption in shale is presented. The adsorption data in shale is generally scarce, therefore, additional capabilities besides the accuracy were considered in the comparison. The multicomponent potential theory of adsorption yields the best results. Moreover, it shows to be useful to extrapolate adsorption data for hydrocarbons that are not available in the literature. An algorithm for phase split calculations considering both capillary pressure and adsorption was developed. The results show that adsorption and capillary pressure can significantly change the phase behavior. In general, a much shrunk phase envelope with a shifted critical point is obtained for hydrocarbon mixtures. Such behavior is mainly caused by compositional changes in the bulk phase due to selective adsorption of the heavier components onto the rock, while the change in bubble point pressure is mainly due to capillary pressure. This study has developed several robust calculation tools for phase equilibrium in porous media with capillary pressure and adsorption effects. Analysis using these tools have shown that capillary pressure and adsorption have non-negligible effects on phase equilibrium in shale. As general tools, they can be used to calculate phase equilibrium in other porous media as well. The compositional simulator with added capillary pressure effects on phase equilibrium can be used for evaluating the effects in dynamic and more complex scenarios.

General information
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Organisations: Center for Energy Resources Engineering, Department of Chemistry, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering
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Projects:
Phase Equilibrium Modeling for Shale Production Simulation
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Phase-Modulated Nonresonant Laser Pulses Can Selectively Convert Enantiomers in a Racemic Mixture
Deracemization occurs when a racemic molecular mixture is transformed into a mixture containing an excess of a single enantiomer. Recent advances in ultrafast laser technology hint at the possibility of using shaped pulses to generate deracemization via selective enantiomeric conversion; however, experimental implementation remains a challenge and has not yet been achieved. Here we suggest a simple, yet novel approach to laser-induced enantiomeric conversion based on dynamic Stark control. We demonstrate theoretically that current laser and optical technology can be used to generate a pair of phase-modulated, nonresonant, linearly polarized Gaussian laser pulses that can selectively deracemize a racemic mixture of 3D-oriented, 3,5-difluoro-3',5'-dibromobiphenyl (F2H3C6-C6H3Br2) molecules, the laser-induced dynamics of which are well studied experimentally. These results strongly suggest that designing a closed-loop coherent control scheme based on this methodology may lead to the first-ever achievement of enantiomeric conversion via coherent laser light in a laboratory setting.

General information
State: Published
Organisations: Department of Chemistry
Authors: Thomas, E. F. (Intern), Henriksen, N. E. (Intern)
Number of pages: 8
Pages: 2212-2219
Publication date: 2017
Plasmon-enhanced Solar Fuel Production with Gold-metal Oxide Hybrid Nanomaterials

Harnessing sunlight to drive chemical reactions for energy storage is an important element in the transition towards green and sustainable technologies. Solar fuel production using semiconductor nanoparticles (SNPs) are widely studied but suffer from poor utilization of the solar spectrum and/or poor stability under operating conditions. A new avenue addressing these challenges involve plasmonic metal nanoparticles (PNPs). These stable materials have tunable optical
properties and exciting catalytic behavior. Composite photocatalysts of SNPs and PNPs exploit the majority of the solar spectrum, provide new catalytic routes and expands the scope of solar photocatalysis. We prepare metal oxide SNPs, gold PNPs and their hybrids through mild aqueous syntheses to develop efficient photocatalyst for solar fuel production. Focus is placed on the synergetic interplay between SNPs and PNPs, understanding the complex pathways, and disentangling plasmon-driven, photothermal and heterogenous catalytic effects.

**General information**
State: Published
Organisations: Department of Chemistry, NanoChemistry, Organic Chemistry, University of California
Authors: Engelbrekt, C. (Intern), Law, M. (Ekstern), Zhang, J. (Intern)
Publication date: 2017
Event: Poster session presented at TMS 2017, San Diego, United States.
Main Research Area: Technical/natural sciences
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Source-ID: 132372202
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**Pressure-induced structural change in liquid GaIn eutectic alloy**
Synchrotron x-ray diffraction reveals a pressure induced crystallization at about 3.4 GPa and a polymorphic transition near 10.3 GPa when compressed a liquid GaIn eutectic alloy up to ~13 GPa at room temperature in a diamond anvil cell. Upon decompression, the high pressure crystalline phase remains almost unchanged until it transforms to the liquid state at around 2.3 GPa. The *ab initio* molecular dynamics calculations can reproduce the low pressure crystallization and give some hints on the understanding of the transition between the liquid and the crystalline phase on the atomic level. The calculated pair correlation function $g(r)$ shows a non-uniform contraction reflected by the different compressibility between the short (1st shell) and the intermediate (2nd to 4th shells). It is concluded that the pressure-induced liquid-crystalline phase transformation likely arises from the changes in local atomic packing of the nearest neighbors as well as electronic structures at the transition pressure.

**General information**
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Organisations: Department of Chemistry, X-ray Crystallography, Zhejiang University, Deutsches Elektronen-Synchrotron
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BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.63 SJR 1.625 SNIP 1.401
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 2.057 SNIP 1.684 CiteScore 5.3
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.103 SNIP 1.544 CiteScore 4.75
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.886 SNIP 1.51 CiteScore 4.06
Probing the global potential energy minimum of (CH$_2$O)$_2$: THz absorption spectrum of (CH$_2$O)$_2$ in solid neon and para-hydrogen

The true global potential energy minimum configuration of the formaldehyde dimer (CH$_2$O)$_2$, including the presence of a single or a double weak intermolecular CH⋯O hydrogen bond motif, has been a long-standing subject among both experimentalists and theoreticians as two different energy minima conformations of C$_s$ and C$_{2v}$ symmetry have almost identical energies. The present work demonstrates how the class of large-amplitude hydrogen bond vibrational motion probed in the THz region provides excellent direct spectroscopic observables for these weak intermolecular CH⋯O hydrogen bond motifs. The combination of concentration dependency measurements, observed isotopic spectral shifts associated with H/D substitutions and dedicated annealing procedures, enables the unambiguous assignment of three large-amplitude infrared active hydrogen bond vibrational modes for the non-planar C$_s$ configuration of (CH$_2$O)$_2$ embedded in cryogenic neon and enriched para-hydrogen matrices. A (semi)-empirical value for the change of vibrational zero-point energy of $5.5 \pm 0.3$ kJ mol$^{-1}$ is proposed for the dimerization process. These THz spectroscopic observations are complemented by CCSD(T)-F12/aug-cc-pV5Z (electronic energies) and MP2/aug-cc-pVQZ (force fields) electronic structure calculations yielding a (semi)-empirical value of $13.7 \pm 0.3$ kJ mol$^{-1}$ for the dissociation energy $D_0$ of this global potential energy minimum.

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Organisations: Department of Chemistry, Technical University of Denmark
Publication date: 2017
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BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.13 SJR 1.073 SNIP 0.755
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.953 SNIP 0.767 CiteScore 1.98
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
We probe the dynamics of valence electrons in photoexcited $\text{[Fe(terpy)$_2$]$^{2+}$}$ in solution to gain deeper insight into the Fe-ligand bond changes. We use hard X-ray emission spectroscopy (XES), which combines element specificity and high penetration with sensitivity to orbital structure, making it a powerful technique for molecular studies in a wide variety of environments. A picosecond-time-resolved measurement of the complete Is X-ray emission spectrum captures the transient photoinduced changes and includes the weak valence-to-core (vtc) emission lines that correspond to transitions from occupied valence orbitals to the nascent core-hole. Vtc-XES offers particular insight into the molecular orbitals directly involved in the light-driven dynamics; a change in the metal ligand orbital overlap results in an intensity reduction and a blue energy shift in agreement with our theoretical calculations and more subtle features at the highest energies.
reflect changes in the frontier orbital populations.

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Organisations: Department of Chemistry, Argonne National Laboratory, Deutsches Elektronen-Synchrotron, European XFEL, Hungarian Academy of Sciences
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BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.48 SJR 1.948 SNIP 1.181
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.917 SNIP 1.268 CiteScore 4.68
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.027 SNIP 1.448 CiteScore 5.08
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 2.134 SNIP 1.439 CiteScore 5.14
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.514 SNIP 1.46 CiteScore 4.98
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.32 SNIP 1.457 CiteScore 4.92
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 2.438 SNIP 1.356
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 2.128 SNIP 1.417
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.856 SNIP 1.033
Web of Science (2008): Indexed yes
Web of Science (2007): Indexed yes
Web of Science (2006): Indexed yes
Web of Science (2005): Indexed yes
Probing ultrafast $\pi^*$/n$\pi^*$ internal conversion in organic chromophores via K-edge resonant absorption

Many photoinduced processes including photosynthesis and human vision happen in organic molecules and involve coupled femtosecond dynamics of nuclei and electrons. Organic molecules with heteroatoms often possess an important excited-state relaxation channel from an optically allowed $\pi^*$ to a dark n$\pi^*$ state. The $\pi^*$n$\pi^*$ internal conversion is difficult to investigate, as most spectroscopic methods are not exclusively sensitive to changes in the excited-state electronic structure. Here, we report achieving the required sensitivity by exploiting the element and site specificity of near-edge soft X-ray absorption spectroscopy. As a hole forms in the n orbital during $\pi^*$n$\pi^*$ internal conversion, the absorption spectrum at the heteroatom K-edge exhibits an additional resonance. We demonstrate the concept using the nucleobase thymine at the oxygen K-edge, and unambiguously show that $\pi^*$n$\pi^*$ internal conversion takes place within (60 +/- 30) fs. High-level-coupled cluster calculations confirm the method’s impressive electronic structure sensitivity for excited-state investigations.

General information
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Organisations: Department of Chemistry, SLAC National Accelerator Laboratory, University of Gothenburg, University of Connecticut, Ecole Polytechnique Federale de Lausanne (EPFL), Uppsala University, Elettra Sincrotrone Trieste
Authors: Wolf, T. J. A. (Ekstern), Myhre, R. H. (Ekstern), Cryan, J. P. (Ekstern), Coriani, S. (Intern), Squibb, R. J. (Ekstern), Battistoni, A. (Ekstern), Berrah, N. (Ekstern), Bostedt, C. (Ekstern), Bucksbaum, P. (Ekstern), Coslovich, G. (Ekstern), Feifel, R. (Ekstern), Gaffney, K. J. (Ekstern), Grijl, J. (Ekstern), Martinez, T. J. (Ekstern), Miyabe, S. (Ekstern), Moeller, S. P. (Ekstern), Mucke, M. (Ekstern), Natan, A. (Ekstern), Obaid, R. (Ekstern), Osipov, T. (Ekstern), Plekan, O. (Ekstern), Wang, S. (Ekstern), Koch, H. (Ekstern), Guehr, M. (Ekstern)
Publication date: 2017
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BFI (2017): BFI-level 2
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BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 11.8 SJR 6.399 SNIP 2.995
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 6.364 SNIP 3.053 CiteScore 11.23
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 6.331 SNIP 3.091 CiteScore 10.77
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 5.967 SNIP 2.776 CiteScore 9.85
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Quantitative NMR Approach to Optimize the Formation of Chemical Building Blocks from Abundant Carbohydrates

The future role of biomass-derived chemicals relies on the formation of diverse functional monomers in high yields from carbohydrates. Recently, it has become clear that a series of α-hydroxy acids, esters and lactones can be formed from carbohydrates in alcohols and water using tin-containing catalysts such as Sn-Beta. These compounds are potential building blocks for polyesters with additional olefin and alcohol functionalities. We employ an NMR approach to identify, quantify and optimize the formation these building blocks in the chemocatalytic transformation of abundant carbohydrates by Sn-Beta. Record yields of the target molecules can be achieved by obstructing competing reactions through solvent choice.

General information
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Organisations: Department of Chemistry, Organic Chemistry, Haldor Topsoe AS
Authors: Elliot, S. G. (Intern), Tolborg, S. (Ekstern), Sádaba, I. (Ekstern), Taarning, E. (Ekstern), Meier, S. (Intern)
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Publication date: 2017
Main Research Area: Technical/natural sciences
Quest of novel GH20 N-acetyl hexosaminidasetransglycosylating catalysts: functional screening, data mining and semi-rational mutagenesis

Lack of access to certain types of oligosaccharides is a severe bottleneck for advances in glycosciences. The transglycosylation activity of retaining glycoside hydrolases (GH) has been used to provide oligosaccharides. The main drawbacks of those enzymes are the competing hydrolysis reaction and the fact that the products are also substrates, thus needing a kinetic control of the reaction. Several approaches have been developed to overcome these, including mechanism modifications (e.g. glycosynthases, chemical rescue), functional screening and data mining to find natural transglycosidases, directed evolution and targeted mutagenesis. Here we focused on N-acetyl hexosaminidas from family GH20 that catalyse removal or addition of GlcNAc and GalNAc. Despite sharing a substrate-assisted mechanism with GH85, for which several glycosynthases have been created, no successful GH20 glycosynthase has been reported. Thus, we turned to discovery and characterization of new GH20s and performing a systematic mutagenesis study. Several new GH20s of bacterial origin were isolated and described by functional screening and data mining, including transglycosidases able to synthesize lacto-N-triose, a valuable oligosaccharide, as well as genuine hydrolases. Mutational analysis of all residues within the catalytic domain which were unchanged in >99% of 371 aligned GH20 sequences was pursued. Indeed, it has been shown that targeting conserved residues increases the likelihood of finding advantageous mutations. Furthermore, it allows for transfer of successful mutations to other GH20s to find new efficient transglycosidases. Notably, even though most conserved residues occur within the first and second shell of substrate interaction, 9 residues inside the (β/α)8 barrel pointing toward the active site are also conserved. To the best of our knowledge, such residues were not studied; although one of them mutated by directed evolution of a GH29 enzyme improved the transglycosylation yield and was transferable to other GH29 members. Here transglycosylation yields of mutants in first shell, second shell and other residues within the (β/α)8 barrel will be compared for GH20.

General information
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Organisations: Department of Biotechnology and Biomedicine, Enzyme and Protein Chemistry, Department of Chemistry, Organic Chemistry, Technical University of Denmark, Aalborg University, University of Copenhagen
Authors: Teze, D. (Intern), Visnapuu, T. (Intern), Kjeldsen, C. (Intern), Duus, J. Ø. (Intern), Cola, C. S. D. (Forskerdatabase), Lie, A. (Forskerdatabase), Pedersen, L. H. (Forskerdatabase), Stougaard, P. (Ekstern), Svensson, B. (Intern)
Publication date: 2017
Event: Abstract from 19th European Carbohydrate Symposium, Barcelona, Spain.
Main Research Area: Technical/natural sciences
Raman detection of hydrohalite formation: Avoiding accidents on icy roads by deicing where salt will not work
The common substance Hydrohalite has a role to play in as diverse areas as Geology, Earth Climatology, Universe Cosmology, and Cryobiology. In this review, the occurrences under very different occasions are described. These relations are not commonly appreciated. During the work, we realized that there is yet an aspect that has been overlooked. Hydrohalite formed sometimes on icy roads resists common salt deicing procedures. Also, hydrohalite can be detected by rather simple Raman spectroscopy instrumentation. It means that it is possible to avoid accidents on icy roads in the following way: Common salt deicing trucks may be equipped with “artificial intelligence” based on a duel deicing system that switches between normal NaCl deicing and non-NaCl deicing based on Raman spectroscopy. The advantages are first of all less traffic accidents and lower environmental impact and corrosion from NaCl, but disadvantages are increased costs of investments and consumption of non-NaCl deicing agents.
Reaction mechanism of dimethyl ether carbonylation to methyl acetate over mordenite: a combined DFT/experimental study

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

General information
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Reagent-Free Electrophoretic Synthesis of Few-Atom-Thick Metal Oxide Nanosheets

Engineering traditional materials into the new form of atomic and free-standing two-dimensional structures is of both fundamental interest and practical significance, but it is in general facing challenges especially for metal oxide semiconductors. We herein report an ultragreen method for the cost-effective and fast preparation of atomic metal oxide nanosheets that can be further transformed into nanofilms. The method combines top-down building block synthesis and bottom-up electrophoretic assembly in water under ambient conditions, using only bulk metal and Milli-Q water without involving any additional reagents. The focus is on free-standing polycrystalline ZnO nanosheets that can be produced with a lateral dimension as large as 10 μm and a thickness of 1 nm (the thinnest free-standing metal oxide nanosheet ever reported). A new electrophoretic assembly mechanism dominated by intrinsic surface polarity was revealed. We also demonstrate potential applications of this approach for wet electronic systems as exemplified by facile and in situ fabrication of dielectric layers and cellular electrets.

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Scopus rating (2016): CiteScore 8.89 SJR 4.114 SNIP 1.905
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Scopus rating (2014): SJR 3.603 SNIP 2.253 CiteScore 8.89
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Relation between molecular electronic structure and nuclear spin-induced circular dichroism

The recently theoretically described nuclear spin-induced circular dichroism (NSCD) is a promising method for the optical detection of nuclear magnetization. NSCD involves both optical excitations of the molecule and hyperfine interactions and, thus, it offers a means to realize a spectroscopy with spatially localized, high-resolution information. To survey the factors relating the molecular and electronic structure to the NSCD signal, we theoretically investigate NSCD of twenty structures of the four most common nucleic acid bases (adenine, guanine, thymine, cytosine). The NSCD signal correlates with the spatial distribution of the excited states and couplings between them, reflecting changes in molecular structure and conformation. This constitutes a marked difference to the nuclear magnetic resonance (NMR) chemical shift, which only reflects the local molecular structure in the ground electronic state. The calculated NSCD spectra are rationalized by means of changes in the electronic density and by a sum-over-states approach, which allows to identify the contributions of the individual excited states. Two separate contributions to NSCD are identified and their physical origins and relative magnitudes are discussed. The results underline NSCD spectroscopy as a plausible tool with a power for the identification of not only different molecules, but their specific structures as well.
Revealing the compact structure of lactic acid bacterial hetero-exopolysaccharides by SAXS and DLS

Molecular structures of exopolysaccharides are required to understand their functions and the relationships between the structure and physical and rheological properties. Small-angle X-ray scattering and dynamic light scattering were used in conjunction with molecular modeling to characterize solution structures of three lactic acid bacterial hetero-exopolysaccharides (HePS-1, HePS-2 and HePS-3). Values of radius of gyration $R_g$, cross-sectional radius of gyration $R_{XS}$, approximate length $L$ and hydrodynamic diameter were not directly proportional to the molar mass and indicated the HePSs adopted a compact coil-like rather than an extended conformation. Constrained molecular modeling of 15,000 randomised HePS-1 conformers resulted in five best-fit structures with $R$ factor of 3.94.6% revealing random coil-like structure. $\Phi$ and $\Psi$ angle analysis of glycosidic linkages in HePS-1 structures suggests Galf residues significantly influence the conformation. Ab initio scattering modeling of HePS-2 and HePS-3 gave excellent curve fittings with $\chi^2$ of 0.43 and 0.34 for best-fit models, respectively, compatible with coil-like conformation. The findings disclose solution behaviour of HePS relevant for their interactions with biomacromolecules e.g. milk proteins.
Rhodium Catalyzed Decarbonylation

Rhodium catalyzed decarbonylation has developed significantly over the last 50 years and resulted in a wide range of reported catalyst systems and reaction protocols. Besides experimental data, literature also includes mechanistic studies incorporating Hammett methods, analysis of kinetic isotope effects as well as computational studies of model systems, which give an indication of the scope of the process. In this chapter, fundamental applications of Rh-catalyzed decarbonylation reactions are surveyed and discussed, including cross-coupling reactions, tandem reactions, and alternative methodologies for process intensification.

General information
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Organisations: Centre for Catalysis and Sustainable Chemistry, Organic Chemistry, Department of Chemistry, Technical University of Denmark
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ROMEO: a new reactor concept for hydroformylation process intensification

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Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry, Friedrich-Alexander University Erlangen-Nuremberg
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Ruthenium-Catalyzed Dehydrogenative Decarbonylation of Primary Alcohols
Dehydrogenative decarbonylation of a primary alcohol involves the release of both dihydrogen and carbon monoxide to afford the one-carbon shorter product. The transformation has now been achieved with a ruthenium-catalyzed protocol by using the complex Ru(COD)Cl$_2$ and the hindered monodentate ligand P(o-tolyl)$_3$ in refluxing p-cymene. The reaction can be applied to both benzylic and long chain linear aliphatic alcohols. The intermediate aldehyde can be observed during the transformation, which is therefore believed to proceed through two separate catalytic cycles involving first dehydrogenation of the alcohol and then decarbonylation of the resulting aldehyde.

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Scopus rating (2016): CiteScore 2.74 SJR 1.133 SNIP 0.653
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.198 SNIP 0.758 CiteScore 2.88
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.181 SNIP 0.767 CiteScore 2.96
Web of Science (2014): Indexed yes
The oxidative dehydrogenation of benzylamine to benzonitrile was studied in batch and continuous flow processes using ruthenium dioxide catalysts with varying ruthenium loadings. Increased conversions were observed in the continuous flow process compared with the batch process (up to 100% in the flow process compared with up to 92% in the batch process), with increased selectivity to benzonitrile (82 and 65%, respectively) and benzonitrile yields (84 and 58%, respectively). The major by-product was N-benzylidenebenzylamine. The ruthenium loading in the catalyst was successfully optimised and the most active catalyst had a ruthenium loading of 2.5-3.5 wt%.

**General information**

State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry
Authors: Nordvang, E. C. (Intern), Schill, L. (Intern), Riisager, A. (Intern), Fehrmann, R. (Intern)
Pages: 1149-1461
N-Acyliminium ions are powerful reactive species for the formation of carbon-carbon and carbon-heteroatom bonds. Strategies relying on intramolecular reactions of N-acyliminium intermediates, also referred to as N-acyliminium ion cyclization reactions, have been employed for the construction of structurally diverse scaffolds, ranging from simple bicyclic skeletons to complex polycyclic systems and natural-product-like compounds. This review aims to provide an overview of cyclization reactions of N-acyliminium ions derived from various precursors for the assembly of structurally diverse scaffolds, covering the literature over the past 12 years (from 2004 to 2015).
Selective Oxidation of Biomass-Derived Chemicals

Due to depleting fossil resources, alternative feedstock for obtaining chemicals is of great importance. Biomass provides a promising alternative renewable carbon source; however, new sustainable processes for conversion of biomass are required to sufficient implementation into the industry. These processes should be able to compete with the established processes based on fossil resources. Glycolaldehyde is an often-observed by-product formed from degradation of larger sugars. Due to competing ecological and economical aspects of the well-established processes for extraction and conversion to chemicals from fossil resources, limited amounts of waste chemicals i.e. by-products are allowed in the processes of conversion of biomass and biomass-derived compounds. It is therefore important to develop methods for conversion of these simple by-products that are environmentally benign and of low cost. The objective of this dissertation was to develop new, alternative and sustainable methods for oxidative catalytic upgrading of biomass-derived compounds, with focus on oxidation of glycolaldehyde and simple alcohols as model substrates for larger sugars. Supported gold nanoparticle were studied for the selective oxidation of glycolaldehyde to glycolic acid, which has found applications in various industries. Limitations by competing reactions and catalyst deactivation was observed, affording up to 68% of glycolic acid at mild and aqueous conditions. The green oxidant, molecular oxygen, was applied for these oxidations and the reaction took place under base-free conditions. Oxidation of glycolaldehyde was further studied in the formation of formic acid. Efficient release of hydrogen from formic acid has proven formic acid a viable precursor for hydrogen, facilitating safe transportation and storage. Hydrogen has found application in various industries including energy conversion by fuel cells. High yields of formic acid was obtained from oxidation of glycolaldehyde over a supported ruthenium catalyst. The effect of the size of the support was studied, however, minor differences was observed. A slightly better yield of formic acid was obtained from nanoparticulate ceria. Vanadium-substituted Keggin polyoxometalates have proven efficient catalysts for conversion of various biomass compounds into formic acid. The Wells-Dawson-type heteropolyoxometalates are less thoroughly studied for biomass conversion. Tungsten-based Wells-Dawson heteropolyoxometalates were synthesized and examined for the oxidation of alcohols and sucrose. However, successful oxidations of the alcohols and sucrose were not observed. The search for application of the synthesized Wells-Dawson heteropolyoxometalate is ongoing in collaboration with the group of Prof. Wasserscheid at FAU in Germany. It was shown, that glycolaldehyde can be selectively converted into glycolic acid or formic acid, depending on the catalyst applied, under mild, aqueous and base-free conditions. High product stability in the ceria-supported ruthenium hydroxide catalyzed oxidation to formic acid, together with the good catalyst activity observed when reusing the catalysts, rendered the developed procedure for formic acid production highly applicable for industrial use. Furthermore, the synthesized Wells-Dawson polyoxometalate catalysts afforded low catalytic oxidative activity.
Shape-selectivity in Biomass Conversion: Zeotype-catalyzed Formation of C₄ Sugars

General information
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Side Effect of Good’s Buffers on Optical Properties of Gold Nanoparticle Solutions
In the search of fluorescent nanoclusters for bioimaging, several synthetic methods have been attempted. Particularly, the formation of gold nanoclusters during synthesis of gold nanoparticles (AuNPs) using Good’s buffers has been achieved. Here 2-(N-morpholino) ethanesulfonic acid (MES), 3-(N-morpholino) propanesulfonic acid (MOPS) and 4-(N-morpholino) butanesulfonic acid (MOBS) are chosen Good’s buffers. Resultant AuNP solutions have been subjected to electrochemical investigations along with UV-vis and fluorescent spectroscopies. Distinct absorption features at ca. 290 and 360 nm and fluorescence emission in range of 350-485 nm are observed in filtrated AuNP-free solutions. Notably, electrochemical oxidation of the buffers generates similar optical properties, suggesting that the degradation products of these compounds contribute significantly to the optical properties in AuNP solutions. This work indicates a need for deeper evaluation of fluorescence signals based on metal nanoparticles or nanoclusters.

General information
State: Published
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Silver-Catalyzed Dehydrogenative Synthesis of Carboxylic Acids from Primary Alcohols
A simple silver-catalyzed protocol has been developed for the acceptorless dehydrogenation of primary alcohols into carboxylic acids and hydrogen gas. The procedure uses 2.5 % Ag₂ CO₃ and 2.5-3 equiv of KOH in refluxing mesitylene to afford the potassium carboxylate which is then converted into the acid with HCl. The reaction can be applied to a variety of benzylic and aliphatic primary alcohols with alkyl and ether substituents, and in some cases halide, olefin, and ester functionalities are also compatible with the reaction conditions. The dehydrogenation is believed to be catalyzed by silver nanoparticles that are formed in situ under the reaction conditions.
Simultaneous modulation of surface composition, oxygen vacancies and assembly in hierarchical Co$_3$O$_4$ mesoporous nanostructures for lithium storage and electrocatalytic oxygen evolution

We developed a facile solution reductive method to simultaneously tune the surface composition, oxygen vacancies and three dimensional assembly in Co$_3$O$_4$ hierarchical nanostructures. The controllable surface composition, oxygen vacancies together with hierarchical micro/nanooarchitectures resulted in superior electrochemical properties when used as the anode materials for lithium-ion batteries and as an electrocatalyst for the oxygen evolution reaction. The excellent electrochemical performance is attributed to the synergistic effects of novel hierarchical morphology, crystal structure of the active materials, the improvement of intrinsic conductivity and inner surface area induced by the oxygen vacancies. The present strategy not only provides a facile method to assemble novel hierarchical architectures, but also paves a way to control surface structures (chemical composition and crystal defects) in other transition-metal compounds, and thus will hold great promise in the fields of energy storage and conversion.
Small-Angle X-ray Scattering Data in Combination with RosettaDock Improves the Docking Energy Landscape

We have performed a benchmark to evaluate the relative success of using small-angle X-ray scattering (SAXS) data as constraints (hereafter termed SAXS\textsubscript{constrain}) in the RosettaDock protocol (hereafter termed RosettaDock\textsubscript{SAXS}). For this purpose, we have chosen 38 protein complex structures, calculated the theoretical SAXS data for the protein complexes using the program CRYSOL, and then used the SAXS data as constraints. We further considered a few examples where crystal structures and experimental SAXS data are available. SAXS\textsubscript{constrain} were added to the protocol in the initial, low-resolution docking step, allowing fast rejection of complexes that violate the shape restraints imposed by the SAXS data. Our results indicate that the implementation of SAXS\textsubscript{constrain} in general reduces the sampling space of possible protein-protein complexes significantly and can indeed increase the probability of finding near-native protein complexes. The methodology used is based on rigid-body docking and works for cases where no or minor conformational changes occur upon binding of the docking partner. In a wider perspective, the strength of RosettaDock\textsubscript{SAXS} lies in the combination of low-resolution structural information on protein complexes in solution from SAXS experiments with protein-protein interaction energies obtained from RosettaDock, which will allow the prediction of unknown three-dimensional atomic structures of protein-protein complexes.

General information
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Organisations: Department of Chemistry, X-ray Crystallography, University of Copenhagen, University of Chicago, CMCassist ApS
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Scopus rating (2014): SJR 1.447 SNIP 1.259 CiteScore 3.88
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Scopus rating (2013): SJR 1.647 SNIP 1.345 CiteScore 4.4
Solvent-Controlled Chemoselectivity in the Photolytic Release of Hydroxamic Acids and Carboxamides from Solid Support

The synthetic utility and theoretical basis of a photolabile hydroxylamine-linker are presented. The developed protocols enable the efficient synthesis and chemoselective photolytic release of either hydroxamates or carboxamides from solid support. The bidetachable mode of the linker unit is uniquely dependent on the solvent. Hydroxamic acids are obtained by performing photolysis in protic solvents, whereas photolysis in aprotic solvents enables the selective release of carboxamides.
Specific Ion Effects in Thermo-Responsive Polymer Solutions

Stimuli-responsive polymers are macromolecules that undergo a significant change in conformation and interactions in response to an external stimulus such as temperature and addition of salts. The applications of these materials are numerous ranging from biomedical applications to fabrication of smart surfaces. The present PhD thesis deals with understanding the fundamentals and mechanisms, which control the physicochemical properties of stimuli-responsive polymers in aqueous saline solutions. The whole study can be divided into two sections: (i) polymers in bulk solution and (ii) polymers adsorbed/grafted to a solid/aqueous interface. The first research approach comprises of three subprojects mainly concerned with understanding the mechanisms through which the salts can affect the polymer stability in solution, an effect that is widely known as the Hofmeister effect. The second research approach includes two subprojects that address adsorption and behavior of homo- and copolymers at solid/aqueous interfaces. Besides understanding the fundamentals of polymer properties at the interfaces, this part aims to indicate how changing the structure of the polymers or addition of salts can affect the structure of the polymer layer. The experimental methods that have been used in this project can also be divided into bulk-related and surface-related measurements. Differential scanning calorimetry was used in order to obtain the phase transition temperature of the polymer solutions, as well as thermodynamics of the transition. Dynamic light scattering was employed to assess the hydrodynamic size of the polymer coils and interchain aggregates. To study adsorption, hydration and conformation of the polymers at the solid/aqueous interfaces, quartz crystal microbalance with dissipation monitoring was used. Ultimately, atomic force microscopy imaging and colloidal probe measurements were conducted to study the topography of the polymer layers and the interactions between the polymer-coated surfaces.

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Organisations: Department of Chemistry
Authors: Moghaddam, S. Z. (Intern), Thormann, E. (Intern)
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S³ HMBC hetero: Spin-State-Selective HMBC for accurate measurement of long-range heteronuclear coupling constants
A novel method, Spin-State-Selective (S³) HMBC hetero, for accurate measurement of heteronuclear coupling constants is introduced. The method extends the S3 HMBC technique for measurement of homonuclear coupling constants by appending a pulse sequence element that interchanges the polarization in 13C-1H methine pairs. This amounts to converting the spin-state selectivity from 1H spin states to 13C spin states in the spectra of long-range coupled 1H spins, allowing convenient measurement of heteronuclear coupling constants similar to other S3 or E.COSY-type methods. As usual in this type of techniques, the accuracy of coupling constant measurement is independent of the size of the coupling constant of interest. The merits of the new method are demonstrated by application to vinyl acetate, the alkaloid strychnine, and the carbohydrate methyl β-maltoside.

General information
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Organisations: Department of Chemistry, Organic Chemistry
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Structural stability of high entropy alloys under pressure and temperature

The stability of high-entropy alloys (HEAs) is a key issue before their selection for industrial applications. In this study, *in-situ* high-pressure and high-temperature synchrotron radiation X-ray diffraction experiments have been performed on three typical HEAs Ni20Co20Fe20Mn20Cr20, Hf25Nb25Zr25Ti25, and Re25Ru25Co25Fe25 (at. %), having face-centered cubic (fcc), body-centered cubic (bcc), and hexagonal close-packed (hcp) crystal structures, respectively, up to the pressure of ∼80 GPa and temperature of ∼1262 K. Under the extreme conditions of the pressure and temperature, all three studied
HEAs remain stable up to the maximum pressure and temperatures achieved. For these three types of studied HEAs, the pressure-dependence of the volume can be well described with the third order Birch-Murnaghan equation of state. The bulk modulus and its pressure derivative are found to be 88.3 GPa and 4 for bcc-Hf\textsubscript{25}Nb\textsubscript{25}Zr\textsubscript{25}Ti\textsubscript{25}, 193.9 GPa and 5.9 for fcc-Ni\textsubscript{20}Co\textsubscript{20}Fe\textsubscript{20}Mn\textsubscript{20}Cr\textsubscript{20}, and 304.6 GPa and 3.8 for hcp-Re\textsubscript{25}Ru\textsubscript{25}Co\textsubscript{25}Fe\textsubscript{25} HEAs, respectively. The thermal expansion coefficient for the three studied HEAs is found to be in the order as follows: fcc-Ni\textsubscript{20}Co\textsubscript{20}Fe\textsubscript{20}Mn\textsubscript{20}Cr\textsubscript{20} ≈ bcc-Hf\textsubscript{25}Nb\textsubscript{25}Zr\textsubscript{25}Ti\textsubscript{25} < hcp-Re\textsubscript{25}Ru\textsubscript{25}Co\textsubscript{25}Fe\textsubscript{25}.

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Organisations: Department of Chemistry, X-ray Crystallography, University of Science and Technology of China, Deutsches Elektronen-Synchrotron, Shenzhen University, Zhejiang University
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Scopus rating (2016): CiteScore 1.72 SJR 0.632 SNIP 0.815
Web of Science (2016): Indexed yes
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Scopus rating (2015): SJR 0.618 SNIP 0.84 CiteScore 1.57
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.005 SNIP 1.18 CiteScore 2.04
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.165 SNIP 1.317 CiteScore 2.24
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.305 SNIP 1.294 CiteScore 2.13
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.373 SNIP 1.318 CiteScore 2.24
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.47 SNIP 1.195
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.518 SNIP 1.238
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.667 SNIP 1.338
Web of Science (2008): Indexed yes
Herein, an effective protocol for solid-phase synthesis of peptidethioalactones by concomitant ring closure and cleavage from the solidsupport is reported. The strategy was applied for mapping the importance of the structural features in *S. schleiferi* AIP (5) by performing an alanine scan and truncation of this natural compound. This furnished some of the most potent inhibitors of accessory gene regulator (agr)-I in the human pathogen *S. aureus* reported to date.
Sulfur ligand mediated electrochemistry of gold surfaces and nanoparticles: what, how, and why

Gold surfaces are widely used in electrochemistry whilst gold nanoparticles have very many uses, with both the surfaces and the particles often being protected by sulfur-bound organic ligands. The ligands not only provide chemical stability but also directly participate in many desired processes. This review considers the diversity of known atomic structures for gold-sulfur interfaces, how these structures facilitate a diversity of mechanisms in electrochemical applications, and why this is possible based on recent advances in the basic understanding of the electronic structure of gold-sulfur bonds. Believed once to be Au(I)-thiolate in character and hence distinctly different to physisorbed thiols and disulfides, chemisorbed bonds are shown to be Au(0)-thiyls instead. A wide range of in-situ STM electrochemical and other data is interpreted from this perspective.
Supercapacitive bioelectrochemical solar cells using thylakoid membranes and carbon nanotubes

Utilization of photosynthetic cell components for light energy harnessing is a perspective tool to achieve a high efficiency of "green" light energy conversion using fully recyclable biomaterials. Inspired by the advantages of recently disclosed concept of simultaneous light energy conversion and storage in the form of electric charge within a singular contrivance, we have developed and investigated supercapacitive photo-bioanodes based on the carboxilized and amidized multwall carbon nanotubes (MWCNTs) in direct electron transfer (DET) communication with adsorbed thylakoid membranes. Employment of the amidized MWCNTs results in higher photo-bioelectrocatalytic current output, lower charge transfer resistance and open circuit potential and higher operational stability compared to the photo-bioanodes based on the carboxilized MWCNTs. The average power density achieved for the optimized supercapacitive photobioelectrochemical cell in a pulse mode was ca. 250 times higher compared to the recent report about the DET-based photo-biosupercapacitor coupled with significantly higher stability and simple design. The findings reported herein disclose new patterns of interactions between the biomaterial and charged surface and may facilitate the development of more efficient, eco-friendly and renewable biological power sources for various application perspective.

General information
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Superionic BioSolar Cell Driven by Direct Electron Transfer between Photosynthetic Membranes and CNT Networks with Enhanced Performance

Integrating photosynthetic cell components with nanostructured materials can facilitate the conversion of solar energy into electric power for creating sustainable carbon-neutral energy sources. With the aim at exploring efficient photoinduced biocatalytic energy conversion systems, we have used an amidated carbon nanotube (aCNT) networked matrix to integrate thylakoid membranes (TM) for construction of a direct electron transfer-driven biosolar cell. We have evaluated the resulting photobioelectrochemical cells systematically. Compared to the carboxylated CNT (cCNT)-TM system, the aCNT-TM system enabled a 1.5-fold enhancement in photocurrent density. This system offers more advantages including a reduced charge-transfer resistance, a lower open-circuit potential, and an improved cell stability. More remarkably, the average power density of the optimized cells was 250 times higher than that of reported analogue systems. Our results suggest the significance of physical and electronic interactions between the photosynthetic components and the support nanomaterials and may offer new clues for designing improved bio solar cells.

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Organisations: Department of Chemistry, NanoChemistry, Organic Chemistry, Lund University, Tambov State Technical University, Malmo University, Novozymes AS
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Superoxide dismutase 1 is positively selected to minimize protein aggregation in great apes
Positive (adaptive) selection has recently been implied in human superoxide dismutase 1 (SOD1), a highly abundant antioxidant protein with energy signaling and antiaging functions, one of very few examples of direct selection on a human protein product (exon); the molecular drivers of this selection are unknown. We mapped 30 extant SOD1 sequences to the recently established mammalian species tree and inferred ancestors, key substitutions, and signatures of selection during the protein's evolution. We detected elevated substitution rates leading to great apes (Hominidae) at ~1 per 2 million years, significantly higher than in other primates and rodents, although these paradoxically generally evolve much faster. The high evolutionary rate was partly due to relaxation of some selection pressures and partly to distinct positive selection of SOD1 in great apes. We then show that higher stability and net charge and changes at the dimer interface were selectively introduced upon separation from old world monkeys and lesser apes (gibbons). Consequently, human, chimpanzee and gorilla SOD1s have a net charge of -6 at physiological pH, whereas the closely related gibbons and macaques have -3. These features consistently point towards selection against the malicious aggregation effects of elevated SOD1 levels in long-living great apes. The findings mirror the impact of human SOD1 mutations that reduce net charge and/or stability and cause ALS, a motor neuron disease characterized by oxidative stress and SOD1 aggregates and triggered by aging. Our study thus marks an example of direct selection for a particular chemical phenotype (high net charge and stability) in a single human protein with possible implications for the evolution of aging.
Surface forces between rough and topographically structured interfaces

Within colloidal science, direct or indirect measurements of surface forces represent an important tool for developing a fundamental understanding of colloidal systems, as well as for predictions of the stability of colloidal suspensions. While the general understanding of colloidal interactions has developed significantly since the formulation of the DLVO theory, many problems still remain to be solved. One concrete problem is that the current theory has been developed for interaction between flat and chemically homogenous surfaces, which is in contrast to the surfaces of most natural and manufactured materials, which possess topographical variations. Further, with technological advances in nanotechnology, fabrication of nano- or micro-structured surfaces has become increasingly important for many applications, which calls for a better understanding of the effect of surface topography on the interaction between interfaces. This paper presents a review of the current state of understanding of the effect of surface roughness on DLVO forces, as well as on the interactions between topographically structured hydrophobic surfaces in water. While the first case is a natural choice because it represents the most general description of colloidal interactions, the second case represents examples of how intentionally built-in surface structures can significantly alter the interactions between surfaces.
Sustainable Chemistry for Biomass Utilization

Vanadium catalyzed deoxydehydration (DODH) of vicinal diols to alkenes have been investigated. The aim of the project was to examine the possibility of using an alcohol as both the solvent and the reductant. Development of a process that functions in a polar solvent was thought to be especially important, as the final goal was to use the method to convert oxygen-rich molecules from biomass into valuable compounds. Initial experiments found the DODH reaction to proceed in an autoclave at 230 °C, when 1,2-decanediol was allowed to react with 5 mol% ammonium metavanadate (NH₄VO₃) in isopropanol. After 17 hours, a yield of 1-decene that corresponded to 50 mol% of the starting substrate, could be detected using gas chromatography. Different alcohols were tested as solvents along with their ability to reduce the vanadium center back to the oxidation state in which it is active. Secondary alcohols gave much better yields than their primary analogues and isopropanol was thus selected for further research. Catalyst optimization was carried out by comparison of the products and yields obtained when a range of different vanadium compounds were used. Most of the screened catalysts gave the same yields and product distributions, and NH₄VO₃ was judged to be a good choice based on its availability and ease of handling. Even though low turn-over numbers were found in batch experiments, the catalyst
proved to be much more sustainable if reused before it gets deactivated. Vanadium catalyzed DODH was found to have unique selectivity towards substrates containing exactly one primary and one secondary hydroxyl group. In contrast, internal diols such as 3,4-hexanediol gave no yield of alkene and both stereoisomers of 1,2-cyclohexanediol were almost completely unreactive. However, substrates that are stabilized by conjugation, such as hydrobenzoin, were found to undergo oxidative cleavage to form two aldehydes. The reactivity of the diols also depends strongly on the orientation of the hydroxyl groups relative to one another. A sharp decline in product yield was thus observed when cis-1,2-cyclohexanediol was added to a reaction of 1,2-hexanediol, which was in contrast to addition of the trans stereoisomer. A possible reason is that the trans isomer cannot simultaneously coordinate to the metal with both hydroxyl groups and thereby inhibit the reaction. Glycerol proved to be unreactive as well, whereas 1,2-propanediol and 3-isopropanediol did undergo DODH to yield propene and 3-isopropano-1-propene, respectively. The water that is formed as the reaction proceeds was found to inhibit the DODH so strongly that removing it might be the key to achieve alkenes yields above 50 mol%. Molecular sieves, 2,2-dimethoxypropane, triethyl orthoformate and various other methods to remove water were tested and analyzed. The vanadium catalyzed reactive distillation of glycerol has also been developed. The reaction setup and conditions were optimized to ensure a quick separation of the products from the mixture. Only 1 mol% NH₄VO₃ was enough to achieve total conversion of 23 g of glycerol, with direct collection of a mixture containing allylic alcohol, acrolein and water. The best results were obtained at 275 °C, with yields of 22 mol% allylic alcohol and roughly 4 mol% acrolein obtained after 5 hours. A black material remained in the reaction flask and its composition was determined by elemental analysis. This material was later proposed to be a polymer mainly built from acrolein and possibly also allylic alcohol and glycerol monomers. The catalytic performance of MeReO₃, (NH₄)₆Mo₇O₂₄·4H₂O and NH₄VO₃ was compared and vanadium found to give more allylic alcohol than rhenium, which is surprising due to the increased DODH reactivity of the latter.
Synthesis and biological evaluation of dihydropyrano-[2,3-c]pyrazoles as a new class of PPARγ partial agonists

Peroxisome proliferator-activated receptor γ (PPARγ) is a well-known target for thiazolidinedione antidiabetic drugs. In this paper, we present the synthesis and biological evaluation of a series of dihydropyrano-[2,3-c]pyrazole derivatives as a novel family of PPARγ partial agonists. Two analogues were found to display high affinity for PPARγ with potencies in the micro molar range. Both of these hits were selective against PPARγ, since no activity was measured when tested against PPARα, PPARδ and RXRα. In addition, a novel modelling approach based on multiple individual flexible alignments was developed for the identification of ligand binding interactions in PPARγ. In combination with cell-based transactivation experiments, the flexible alignment model provides an excellent analytical tool to evaluate and visualize the effect of ligand chemical structure with respect to receptor binding mode and biological activity.

General information
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Synthesis and characterization of iron-cobalt (FeCo) alloy nanoparticles supported on carbon

Iron-cobalt nanocrystalline bimetallic alloys supported on carbon microparticles were synthesized and characterized. The preparation methods involved the use of iron and cobalt chloride or acetate precursor salts in water and direct co-precipitation or wet impregnation techniques. The size of the alloy nanoparticles differed depending on the preparation method. When the wet impregnation technique of acetate precursor salts of Fe and Co were used for the synthesis, the size of FeCo alloy nanoparticles was approximately 13 nm. FeCo alloy nanoparticles were characterized by crystallography (XRD), thermogravimetric analysis (TGA), electron microscopy, energy dispersive X-ray spectroscopy analysis (EDX), and atomic force microscopy (AFM). In all cases, we observed well-dispersed nanometer size alloy particles on the surface of carbon microparticles. FeCo supported on such carbon microparticles are chemically and mechanically stable for prolonged periods of time. AFM analysis showed that the FeCo nanoparticles were formed on the surface of the carrier. The results of this study suggest that using these easy and inexpensive synthetic methods iron-cobalt nanoparticles can be formed on carbon microparticles support materials with applications in catalysis, microelectronics, and biomedicine
Synthesis and Development of Diagnostic Tools for Medical Imaging

The need for novel diagnostic tools in medical imaging is increasing since they can improve the positive therapeutic outcome as well as patient compliance. In this thesis different diagnostic tools were developed within an interdisciplinary project, whereas the main work reported in this thesis was the synthesis of different materials. The first project introduces the development of injectable fiducial markers within the field of image-guided radiotherapy. Fiducial markers for computed tomography (CT)-imaging are today needed in order to correlate the positioning of the tumor to provide a more precise and improved radiation, as tumors rarely display a fixed position during radiotherapy. A fiducial marker based on encapsulated gold nanoparticles within the gelation matrix of sucrose acetate isobutyrate (SAIB) was developed and tested in vivo. The scientific objective was to provide sufficient surface engineering of the gold nanoparticles that will allow full dispersion of AuNPs within the hydrophobic environment of the SAIB matrix. As stabilizing coating-materials PEG, PNIPAM polymers and a dithiolane SAIB derivative were tested. The unique gelation properties of the SAIB matrix led to the second project of injectable fiducial tissue markers for surgical guidance of non-palpable tumors and brachytherapy. As radioactive tracer, radioiodinated SAIB-derivatives were developed based on the regioselective ipso-iodination of aryl-TMS moieties. Radioiodination was conducted under carrier free conditions in high radiochemical yields by Tl(OOCCF$_3$)$_3$ and [125I]NaI. The application of the radioabeled 125I-SAIB derivative was tested in vivo as a tissue marker for surgical guidance and evaluated in terms of dosimetry. The third project involved the synthesis of iodide-based contrast agents designed for remote loading of liposomes. Long circulating contrast agents for blood pool imaging by CT-imaging are of
interest due to the current limitations of short retention times and the considerable amounts needed to achieve a proper contrast. A small library of contrast agents designed for remote loading of liposomes was synthesized. Remote loading of one candidate was successful; however, the proper contrast level was not sufficient to be visible by CT-imaging. Another diagnostic tool for blood pool imaging is DOTA-modified pluronic/cyclodextrin (CD)-based polyrotaxanes (PRs). With the previously reported chelation of Gd and the prolonged retention time of Gd-chelated Pluronic/CD PRs, the aim was to extend the use of DOTA-modified Pluronic/CD-based PRs for positron emitting agents by chelation of $^{64}$Cu. Pluronic/CD-based PRs grafted with DOTA was synthesized in the fourth project. The last project deals with the site-specific radiiodination of peptides and proteins. To achieve a conclusive outcome in radioimmunoassays as well as retaining a high binding affinity of receptor binding peptides, the regioselective radiiodination is crucial. Therefore, a TMS-substituted tyrosine was synthesized via the Negishi coupling to test if regioselective iodination could be obtained. The tyrosine derivative was used in the synthesis of dipeptides of phenylalanine, tyrosine and tryptophan respectively in order to evaluate the selectivity towards the ipso-substitution of the TMS in the iodination reaction. First proof-of-concept experiments using aryl-TMS as placeholder in the site-specific iodination of peptides and proteins have been demonstrated.

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**Synthesis and formulation studies of griseofulvin analogues with improved solubility and metabolic stability**
Griseofulvin (1) is an important antifungal agent that has recently received attention due to its antiproliferative activity in mammalian cancer cells. Comprehensive SAR studies have led to the identification of 2′-benzylamino griseofulvin 2, a more potent analogue with low micromolar anticancer potency in vitro. Analogue 2 was also shown to retard tumor growth through inhibition of centrosomal clustering in murine xenograft models of colon cancer and multiple myeloma. However, similar to griseofulvin, compound 2 exhibited poor metabolic stability and aqueous solubility. In order to improve the poor pharmacokinetic properties, 11 griseofulvin analogues were synthesized and evaluated for biological activity and physiological stabilities including SGF, plasma, and metabolic stability. Finally, the most promising compounds were investigated in respect to thermodynamic solubility and formulation studies. The 2′-benzylamine analogue 10 proved to be the most promising compound with low μM in vitro anticancer potency, a 200-fold increase in PBS solubility over compound 2, and with improved metabolic stability. Furthermore, this analogue proved compatible with formulations suitable for both oral and intravenous administration. Finally, 2′-benzylamine analogue 10 was confirmed to induce G2/M cell cycle arrest in vitro.

**General information**
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We report here the direct formation of the new chemical product, trans-2,5-dihydroxy-3-pentenoic acid methyl ester, from pentoses using tin-containing silicates as catalysts. The product is formed under alkali-free conditions in methanol at temperatures in the range 140–180 °C. The highest yields are found using Sn-Beta as the catalyst. Under optimised conditions, a yield of 33% is achieved. Purified trans-2,5-dihydroxy-3-pentenoic acid methyl ester was used for copolymerisation studies with ethyl 6-hydroxyhexanoate using Candida antarctica Lipase B as the catalyst. The copolymerisation yields a product containing functional groups originating from trans-2,5-dihydroxy-3-pentenoic acid methyl ester in the polyester backbone. The reactivity of the incorporated olefin and hydroxyl moieties was investigated using trifluoroacetic anhydride and thiol-ene chemistry, thus illustrating the potential for functionalising the new copolymers.

Synthesis of a novel polyester building block from pentoses by tin-containing silicates

We report here the direct formation of the new chemical product, trans-2,5-dihydroxy-3-pentenoic acid methyl ester, from pentoses using tin-containing silicates as catalysts. The product is formed under alkali-free conditions in methanol at temperatures in the range 140–180 °C. The highest yields are found using Sn-Beta as the catalyst. Under optimised conditions, a yield of 33% is achieved. Purified trans-2,5-dihydroxy-3-pentenoic acid methyl ester was used for copolymerisation studies with ethyl 6-hydroxyhexanoate using Candida antarctica Lipase B as the catalyst. The copolymerisation yields a product containing functional groups originating from trans-2,5-dihydroxy-3-pentenoic acid methyl ester in the polyester backbone. The reactivity of the incorporated olefin and hydroxyl moieties was investigated using trifluoroacetic anhydride and thiol-ene chemistry, thus illustrating the potential for functionalising the new copolymers.

General information
Synthesis of arabinoxylan fragments

The cell wall of plants can be termed the skeleton of the plant. One of the parts making up the cell wall is hemicellulose. Hemicellulose is composed of a number of saccharides where one of the most abundant are the arabinoxylan-oligosaccharides. In many instances the biosynthesis and degradation of arabinoxylan oligosaccharides remain elusive. As a consequence defined arabinoxylan fragments have been chosen as synthetic targets which subsequently will be submitted to enzymatic studies. A better understanding of these processes could lead to e.g. better utilisation of the biomass for biofuel production, or production of commercial chemicals which are mainly obtained from fossil fuels today. The arabinoxylan fragments have a backbone of β-1,4-linked xylans with α-L-arabinose units attached at specific positions. The synthesis utilises an efficient synthetic route, where all the xylan units can be derived from D-xylose through a common intermediate. The xylose units feature the same thiophenyl donor functionality to allow for successive coupling with the same optimised glycosylation protocol. Then, the arabinose units can be attached and global deprotection yields the target fragments.
Synthesis of branched–backbone oligosaccharides of the pectic RG-I plant cell wall polysaccharide

Plants are an essential part of life on earth. They are the primary food producers, climate regulators and provide habitats for other organisms. The dependence of industrialized nations on plant cell walls due to their industrial applications has rapidly increased. Cellulose, hemicelluloses, and pectin polysaccharides are the main structural components of the plant cell wall. Among plant carbohydrates, pectins are highly heterogeneous polysaccharides. They are mainly found in the primary plant cell wall and contribute to various cell functions, including support, defense, signaling, and cell adhesion. Rhamnogalacturonan I (RG-I) is one of the structural classes of pectic polysaccharides, along with homogalacturonan, rhamnogalacturonan II, and xylogalacturonan. The chemical structure of RG-I is complex having a backbone consisting of alternating α-linked L-rhamnose and D-galacturonic acid units with numerous branches of galactan, arabinan, or arabinogalactan positioned at C-4 of the rhamnose residues. The use of defined oligosaccharides rather than isolated polysaccharides can aid in obtaining detailed information about biosynthetic pathways, plant evolution, and agronomical properties. Furthermore, biological testing can provide new insight into plant biology; important for plant preservation, engineering, and utilization of plants as a source of bioenergy. Present work towards defined RG-I substructures involves [4+3]-coupling to furnish a heptasaccharide backbone unit (see Figure 1). Moreover, installation of sidechains of different lengths and nature can be installed at the C-4 position of rhamnose unit. Finally, these oligosaccharides will be deprotected to furnish target molecules to pursue biological studies.

Synthesis of mixed-linked xylans for enzyme characterization

The study of plant cell wall polysaccharides and their corresponding interactions with proteins is vital to get new insights into plant development. Moreover, these polysaccharides are of interest in biotechnological research, due to their use in numerous industrial applications such as food, healthcare and sustainable biofuel production. A major class of hemicellulose is arabinoxylan that is an important polysaccharide component of lignocellulosic biomass. To underpin the full commercial exploitation of these glycan polymers, it is necessary to learn more about the enzymatic hydrolysis of arabinoxylans. This can be achieved by chemical synthesis of well-defined oligosaccharides as models for the more complex macromolecules. Moreover, the utilization of enzyme resistant substrates can support the mapping of the active site of glycosyl-hydrolases. The talk will highlight the synthesis of mixed O- and S-linked tetraxylans as possible interesting candidates for the investigation and characterization of arabinoxylan degrading enzymes.

Synthesis of plant cell wall oligosaccharides

Plant cell walls are structurally complex and contain a large number of diverse carbohydrate polymers. These plant fibers are a highly valuable bio-resource and the focus of food, energy and health research. We are interested in studying the
interplay of plant cell wall carbohydrates with proteins such as enzymes, cell surface lectins, and antibodies. However, detailed molecular level investigations of such interactions are hampered by the heterogeneity and diversity of the polymers of interest. To circumvent this, we target well-defined oligosaccharides with representative structures that can be used for characterizing protein-carbohydrate binding. The presentation will highlight chemical syntheses of plant cell wall oligosaccharides from the group and provide examples from studies of their interactions with proteins.

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### Synthetic Applications and Mechanistic Studies of the Hydroxide-Mediated Cleavage of Carbon-Carbon Bonds in Ketones

The hydroxide-mediated cleavage of ketones into alkanes and carboxylic acids has been reinvestigated and the substrate scope extended to benzyl carbonyl compounds. The transformation is performed with a 0.05 M ketone solution in refluxing xylene in the presence of 10 equiv of potassium hydroxide. The reaction constitutes a straightforward protocol for the synthesis of certain phenyl-substituted carboxylic acids from 2-phenylcycloalkanones. The mechanism was investigated by kinetic experiments which indicated a first order reaction in hydroxide and a full negative charge in the rate-determining step. The studies were complemented by a theoretical investigation where two possible pathways were characterized by DFT/M06-2X. The calculations showed that the scission takes place by nucleophilic attack of hydroxide on the ketone followed by fragmentation of the resulting oxyanion into the carboxylic acid and a benzyl anion.

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Synthetic Nucleic Acid Analogues in Gene Therapy: An Update for Peptide–Oligonucleotide Conjugates

The main objective of this work is to provide an update on synthetic nucleic acid analogues and nanoassemblies as tools in gene therapy. In particular, the synthesis and properties of peptide–oligonucleotide conjugates (POCs), which have high potential in research and as therapeutics, are described in detail. The exploration of POCs has already led to fruitful results in the treatment of neurological diseases, lung disorders, cancer, leukemia, viral, and bacterial infections. However, delivery and in vivo stability are the major barriers to the clinical application of POCs and other analogues that still have to be overcome. This review summarizes recent achievements in the delivery and in vivo administration of synthetic nucleic acid analogues, focusing on POCs, and compares their efficiency.
Ten Challenges of the Amyloid Hypothesis of Alzheimer's Disease

The inability to effectively halt or cure Alzheimer's disease (AD), exacerbated by the recent failures of high-profile clinical trials, emphasizes the urgent need to understand the complex biochemistry of this major neurodegenerative disease. In...
this paper, ten central, current challenges of the major paradigm in the field, the amyloid hypothesis, are sharply formulated. These challenges together show that new approaches are necessary that address data heterogeneity, increase focus on the proteome level, use available human patient data more actively, account for the aging phenotype as a background model of the disease, unify our understanding of the interplay between genetic and non-genetic risk factors, and combine into one framework both the familial and sporadic forms of the disease.

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Scopus rating (1999): SJR 0.228 SNIP 0.448
The A Priori Design and Selection of Ionic Liquids as Solvents for Active Pharmaceutical Ingredients

In this paper we derive a straightforward computational approach to predict the optimal ionic liquid (IL) solvent for a given compound, based on COSMO-RS calculations. These calculations were performed on 18 different active pharmaceutical ingredients (APIs) using a matrix of 210 hypothetical ILs. These results indicated that the 18 APIs could be classified into three distinct categories based on their relative hydrogen bond donating or accepting ability, with similar optimal IL solvent predictions within each class. Informed by these results, a family of strongly hydrogen bond donating ILs based on the N-alkylguanidinium cation were prepared and characterized. The solubility of the APIs in each of these classes was found to be qualitatively consistent with the predictions of the COSMO-RS model. The suitability of these novel guanidinium salts as crystallization solvents was demonstrated by the use of N-butylguanidinium bis(trifluoromethanesulfonyl)imide for the purification of crude fenofibrate using dimethylsulfoxide as an antisolvent, which resulted in good yields and excellent purities. Finally, a simple descriptor based model is proposed to suggest the best IL solvent for arbitrary APIs.

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry, Auckland University of Technology, McGill University, Massachusetts Institute of Technology
Authors: Kunov-Kruse, A. J. (Intern), Weber, C. C. (Ekstern), Rogers, R. D. (Ekstern), Myerson, A. S. (Ekstern)
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BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 5.03 SJR 2.247 SNIP 1.046
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 2.416 SNIP 1.184 CiteScore 4.99
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.487 SNIP 1.219 CiteScore 5.51
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.604 SNIP 1.239 CiteScore 5.68
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 2.884 SNIP 1.294 CiteScore 5.55
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 2.726 SNIP 1.336 CiteScore 5.46
The Au-S bond in biomolecular adsorption and electrochemical electron transfer

Interfacial electrochemical electron transfer (ET) of redox metalloproteins is long established. For the proteins to retain full ET or enzyme activity, modification of the electrode surfaces, such as gold surfaces by self-assembled molecular monolayers (SAMs), is nearly always required, where pure and functionalized alkanethiols have emerged as core linkers. We overview first binding and single-molecule long-range electron transfer of some metalloproteins, metalloenzymes, and DNA-based molecules on single-crystal Au(111), Au(100), and Au(100) electrode surfaces, bound either directly by Au-S linking of surface cysteines to the gold surfaces, or indirectly by non-covalent linking to SAMs of pure and functionalized alkanethiols. Core techniques are electrochemistry, surface spectroscopies, and in situ STM and AFM under electrochemical potential control, framed by single-molecule charge transport theory and electronic structure computations. Molecular packing, voltammetry and in situ STM/AFM are found to be exceedingly sensitive to the structure of the thiol-based SAM molecules, testifying both to the crucial importance of the Au-S binding, and to the SAM linking to the protein. A primary focus that has emerged is the electronic structure of the Au-S link and the packing of the SAMs. We have, first disentangled a wealth of data to identify the nature of the core Au-S contact. All data suggest that the electronic Au-S link is dominated by a Au(0)-thiyl radical with strong vander Waals forces and not by a Au(I)-thiolate ionic/covalent unit. Molecular packing is, further crucially determined by the SAM molecular structure and involves binding either to Au-atoms mined out of the surface or directly to a flat single-crystal surface. We illustrate this by high-resolution in situ STM of straight, branched, and chiral alkanethiols on Au(111)-electrode surfaces.
The importance of V.G. Levich's research in the development of modern electrochemistry

The fundamental scientific areas founded and developed by V.G. Levich and his school, and their importance in contemporary theoretical electrochemistry have been overviewed.

General information
State: Published
Organisations: Department of Chemistry, NanoChemistry, Lomonosov Moscow State University, Russian Academy of Sciences
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Pages: 893-896
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Main Research Area: Technical/natural sciences

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ISSN (Print): 1023-1935
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BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 0.86
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 0.73
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 0.74
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 0.63
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 0.52
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 0.45
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
BFI (2008): BFI-level 1
Web of Science (2007): Indexed yes
Web of Science (2006): Indexed yes
Web of Science (2004): Indexed yes
Web of Science (2003): Indexed yes
Web of Science (2002): Indexed yes
Web of Science (2001): Indexed yes
Original language: English
The influence of different linker modifications on the catalytic activity and cellulose affinity of cellobiohydrolase Cel7A from Hypocrea jecorina

Various cellulases consist of a catalytic domain connected to a carbohydrate-binding module (CBM) by a flexible linker peptide. The linker is often strongly O-glycosylated and typically has a length of 20-50 amino acid residues. Functional roles, other than connecting the two folded domains, of the linker and its glycans, have been widely discussed, but experimental evidence remains sparse. One of the most studied cellulose degrading enzymes is the multi-domain cellobiohydrolase Cel7A from Hypocrea jecorina. Here, we designed variants of Cel7A with mutations in the linker region to elucidate the role of the linker. We found that moderate modification of the linker could result in significant changes in substrate affinity and catalytic efficacy. These changes were quite different for different linker variants. Thus, deletion of six residues near the catalytic domain had essentially no effects on enzyme function. Conversely, a substitution of four glycosylation sites near the middle of the linker reduced substrate affinity and increased maximal turnover. The observation of weaker binding provides some support of recent suggestions that linker glycans may be directly involved in substrate interactions. However, a variant with several inserted glycosylation sites near the CBM also showed lower affinity for the substrate compared to the wild-type, and we suggest that substrate interactions of the glycans depend on their exact location as well as other factors such as changes in structure and dynamics of the linker peptide.
The Manganese-Catalyzed Cross-Coupling Reaction and the Influence of Trace Metals

The substrate scope of the MnCl₂-catalyzed cross-coupling between aryl halides and Grignard reagents has been extended to several methyl-substituted aryl iodides by performing the reaction at elevated temperature in a microwave oven. A radical clock experiment revealed the presence of an aryl radical as an intermediate leading to the proposal of an S_{RN1} pathway for the coupling. The mechanistic information gave rise to suspicion about two previously published cross-coupling reactions catalyzed by manganese(II) salts. As a result, the coupling between aryl halides and organostannanes as well as between aryl halides and amines were revisited. Both reactions were found impossible to reproduce without the addition of small amounts of palladium or copper and are therefore not believed to be catalyzed by manganese.

General information

State: Published
Organisations: Department of Chemistry, Organic Chemistry, Technical University of Denmark, University of Gothenburg
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Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.74 SJR 1.133 SNIP 0.653
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
The Pathogenic A2V Mutant Exhibits Distinct Aggregation Kinetics, Metal Site Structure, and Metal Exchange of the Cu²⁺-Aβ Complex

A prominent current hypothesis is that impaired metal ion homeostasis may contribute to Alzheimer's disease (AD). We elucidate the interaction of Cu²⁺ with wild-type (WT) Aβ₁₋₄₀ and the genetic variants A2T and A2V which display increasing pathogenicity as A2T<WT<A2V. Cu²⁺ significantly extends the lag phase in aggregation kinetics, in particular for the pathogenic A2V variant. Additionally, a rapid, initial, low intensity ThT response is observed, possibly reflecting formation of Cu²⁺-induced amorphous aggregates, as supported by atomic force microscopy (AFM) and circular dichroism (CD) spectroscopy, again most notably for the A2V variant. Electron paramagnetic resonance (EPR) spectroscopy gives p
$K_a$ values for transition between two Cu$^{2+}$ coordination geometries (component I and II) of 7.4 (A2T), 7.9 (WT), and 8.4 (A2V), that is, component I is stabilized at physiological pH in the order A2T<WT<A2V. $^1$H NMR relaxation exhibits the same trend for the non-coordinating aromatic residues (A2T<WT<A2V), and implies markedly faster inter-peptide Cu$^{2+}$ exchange for the A2V variant than for WT and A2T. We therefore hypothesize that component I of the Cu–Aβ complex is related to pathogenicity, accounting for both the pathogenic nature of the A2V variant and the protective nature of the A2T variant.
Thermodynamic Analysis of Chalk–Brine–Oil Interactions

The surface complexation models (SCMs) are used successfully for describing the thermodynamic equilibrium between the pure calcite surface (carbonate and calcium sites) and brine solutions. In this work, we show that the model parameters that are reported for the calcite–brine system are not applicable to the natural carbonates. We adjust the SCM reaction equilibrium constants by fitting the model to the ζ potential data that are reported for the pulverized Stevns Klint chalk. Then, we use the model, implemented in the PhreeqcRM geochemistry package coupled with a finite volume solver, to predict the breakthrough composition of different ions in the chromatographic experiments on the intact Stevns Klint chalk cores. Again, the model falls short in predicting the reactive transport of brine in a natural carbonate, implying that ζ potential data is not enough for optimizing the SCM model parameters for the reactive transport applications. We propose an optimization procedure that fits the coupled SCM–transport model parameters to the chromatographic (single-phase core flooding) data. The ζ potential measurements are implemented in the optimization scheme as nonlinear constraints. We then use the optimized model to study the thermodynamic equilibrium between the oil and chalk surfaces in the presence of different brine compositions, including the dissolution and precipitation of minerals. We represent the chalk–oil interactions by acid–base equilibrium reactions between the calcium and carbonate sites on the chalk surface and carboxylic acids and amine bases on the oil surface, respectively. Comparing the model results to a data set of the spontaneous imbibition experiments for chalk shows that the remaining oil saturation in the imbibition experiments is correlated with the number of bonds between the amine and carboxylate groups on the oil surface and the carbonate and protonated calcium on the chalk surface.

General information
State: Published
Organisations: Centre for oil and gas – DTU, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Ressources Engineering, Department of Chemistry
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Pages: 11773–11782
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Main Research Area: Technical/natural sciences

Publication information
Journal: Energy and Fuels
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BFI (2018): BFI-level 2
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Thermodynamic modelling of acid gas removal from natural gas using the Extended UNIQUAC model

Thermodynamics of natural gas sweetening process needs to be known for proper design of natural gas treating plants. Absorption with aqueous N-Methyldiethanolamine is currently the most commonly used process for removal of acid gas (CO₂ and H₂S) impurities from natural gas. Model parameters for the Extended UNIQUAC model have already been determined by the same authors to calculate single acid gas solubility in aqueous MDEA. In this study, the model is further extended to estimate solubility of CO₂ and H₂S and their mixture in aqueous MDEA at high pressures with methane as a makeup gas.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Department of Chemistry, CERE – Center for Energy Resources Engineering
Thermo-responsive diblock and triblock cationic copolymers at the silica/aqueous interface: A QCM-D and AFM study
The properties of synthesized diblock poly(N-isopropylacrylamide)-poly[(3-acrylamidopropyl)trimethylammonium chloride] and triblock methoxy-poly(ethylene glycol)-poly(N-isopropylacrylamide)-poly[(3-acrylamidopropyl)trimethylammonium chloride] cationic copolymers at the silica/aqueous interface are investigated using quartz crystal microbalance with dissipation monitoring (QCM-D) and atomic force microscopy (AFM). Moreover, dynamic light scattering is employed to assess the copolymers in terms of the hydrodynamic size and interchain aggregation. Although viscoelastic Voigt modeling of the QCM-D data suggests a comparable layer thickness for the copolymers on the silica surface, the AFM imaging and colloidal probe measurements reveal significant differences in surface coverage and thickness of the layers, which are discussed and compared with respect to the stabilization effect by the hydrophilic poly(ethylene glycol) block.

General information
State: Published
Organisations: Department of Chemistry, University of Oslo
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Pages: 546-555
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Main Research Area: Technical/natural sciences

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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.14 SJR 1.144 SNIP 1.267
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.095 SNIP 1.263 CiteScore 3.8
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.166 SNIP 1.406 CiteScore 3.74
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.19 SNIP 1.45 CiteScore 3.73
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.298 SNIP 1.469 CiteScore 3.4
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
The structure of Lactococcus lactis thioredoxin reductase reveals molecular features of photo-oxidative damage

The NADPH-dependent homodimeric flavoenzyme thioredoxin reductase (TrxR) provides reducing equivalents to thioredoxin, a key regulator of various cellular redox processes. Crystal structures of photo-inactivated thioredoxin reductase (TrxR) from the Gram-positive bacterium Lactococcus lactis have been determined. These structures reveal novel molecular features that provide further insight into the sensitivity of this enzyme toward visible light. We propose that a pocket on the si-face of the isoalloxazine ring accommodates oxygen that reacts with photo-excited FAD generating superoxide and a flavin radical that oxidize the isoalloxazine ring C7α methyl group and a nearby tyrosine residue. This tyrosine and key residues surrounding the oxygen pocket are conserved in enzymes from related bacteria, including pathogens such as Staphylococcus aureus. Photo-sensitivity may thus be a widespread feature among bacterial TrxR with the described characteristics, which affords applications in clinical photo-therapy of drug-resistant bacteria.

General information
State: Published
Organisations: Department of Biotechnology and Biomedicine, Department of Chemistry, X-ray Crystallography, Enzyme and Protein Chemistry, Department of Systems Biology, Enzyme and Protein Chemistry, University of Copenhagen
Authors: Skjoldager, N. (Intern), Bang, M. B. (Intern), Rykær, M. (Intern), Björnberg, O. (Intern), Davies, M. J. (Ekstern), Svensson, B. (Intern), Harris, P. (Intern), Hägglund, P. (Intern)
Number of pages: 10
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The ternary Fe-C-N system: Homogeneous distributions of nitrogen and carbon

Porous iron foils were used for synthesizing homogeneous samples of iron carbides and (carbo)nitrides. Homogeneous distributions of interstitial nitrogen and carbon were obtained without long treatment times due to limited required diffusion distances in the porous material. By adjustments of the nitriding and carburizing potentials, tailored nitrogen and carbon contents can be achieved, which allows assessment of a phase stability diagram for the Fe-N-C system, for which available experimental data is limited. Thermal decomposition sequences were established for the various iron carbides and (carbo)nitrides using in situ synchrotron X-ray diffraction. Hägg carbide (χ) and ε-carbonitride, Fe$_2$(N,C)$_{1-z}$, with high carbon content decompose to cementite (θ) above 850 K, while ferrite (α) forms above 950 K and austenite (γ) above 1025 K. For high nitrogen contents ζ-Fe$_2$(N,C) is transformed to ε from 680 to 770 K, which decomposes to γ′-Fe$_4$(N,C)$_{1+x}$ between 795 and 900 K as nitrogen is released as N$_2$. Ferrite forms above 850 K while austenite may be briefly formed around 900 K. The two iron carbides, cementite and Hägg carbide, exhibit different coefficients of thermal expansion. Below approximately 480 K, cementite is ferromagnetic and a volumetric thermal expansion coefficient of α$_V$ = 1.5 × 10$^{-5}$ K$^{-1}$ is obtained. The average value in the paramagnetic state is α$_V$ = 4.3 (3) × 10$^{-5}$ K$^{-1}$. For Hägg carbide the average value is α$_V$ = 3.8 (5) × 10$^{-5}$ K$^{-1}$ and only a minor change in unit cell volume is observed at the magnetic transition temperature.

General information
State: Published
Organisations: Department of Mechanical Engineering, Materials and Surface Engineering, Department of Chemistry, X-ray Crystallography
Authors: Brink, B. (Intern), Ståhl, K. (Intern), Christiansen, T. L. (Intern), Somers, M. A. J. (Intern)
Thiosemicarbazone organocatalysis: Tetrahydropyranylation and 2-deoxygalactosylation reactions and kinetics-based mechanistic investigation

The first use of thiosemicarbazone-based organocatalysis was demonstrated on both tetrahydropyranylation and 2-deoxygalactosylation reactions. The organocatalysts were optimised using kinetics-based selection. The best catalyst outperformed previously reported thiourea catalysts for tetrahydropyranylation by 50-fold. Hammett investigations of both the organocatalyst and the substrate indicate an oxyanion hole-like reaction mechanism.

General information
State: Published
Organisations: Department of Chemistry, University of Copenhagen
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Number of pages: 5
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 8.44 SJR 4.475 SNIP 1.67
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 4.74 SNIP 1.749 CiteScore 9.13
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 4.991 SNIP 1.745 CiteScore 8.99
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 4.675 SNIP 1.587 CiteScore 8.44
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 5.146 SNIP 1.819 CiteScore 8.18
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 4.33 SNIP 1.799 CiteScore 7.01
ISI indexed (2011): ISI indexed no
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Time-resolved X-ray scattering by electronic wave packets: analytic solutions to the hydrogen atom

Modern pulsed X-ray sources permit time-dependent measurements of dynamical changes in atoms and molecules via non-resonant scattering. The planning, analysis, and interpretation of such experiments, however, require a firm and elaborated theoretical framework. This paper provides a detailed description of time-resolved X-ray scattering by non-stationary electronic wave packets in atomic systems. A consistent application of the Waller-Hartree approximation is discussed and different contributions to the total differential scattering signal are identified and interpreted. Moreover, it is demonstrated how the scattering signal of wave packets in the hydrogen atom can be expressed analytically. This permits simulations without numerical integration and establishes a benchmark for both efficiency and accuracy. Based on that, scattering patterns of an exemplary wave packet in the hydrogen atom are computed for different points in time. In doing so, distinct features of time-resolved X-ray scattering by non-stationary electronic wave packets are illustrated and accentuated in greater detail than it has been done before.

General information
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Organisations: Department of Chemistry
Authors: Simmermacher, M. (Intern), Henriksen, N. E. (Intern), Møller, K. B. (Intern)
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BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.06 SJR 1.678 SNIP 1.117
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.771 SNIP 1.244 CiteScore 4.45
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.772 SNIP 1.253 CiteScore 4.29
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.715 SNIP 1.216 CiteScore 4.05
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.916 SNIP 1.184 CiteScore 3.67
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.697 SNIP 1.203 CiteScore 3.6
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.802 SNIP 1.196
Towards the Synthesis of Diverse Types of Carrageenan Oligosaccharides

Carrageenans are a family of linear sulfated polysaccharides that are extracted from red seaweeds. They play important roles in the biology of algae and furthermore they have many important industrial applications, such as gelling agent in the food industry. The idealized structures of the 10 known types of carrageenans are presented in Figure 1. The carrageenans are intriguing structures: they have a backbone of D-galactose with alternating β-1,4 and α-1,3 bonds with varying degree of sulfation of the 2, 6, 2’ and 4’-positions. Upon treatment with alkali, an 1,3-anhydrogalactose is formed and the α-linked galactose residues undergo a conformational change from 4C1 to 1C4 which increases the gelling property of the molecule. We wish to synthesize well-defined oligocarrageenans. Our synthetic strategy aims at producing all ten types of carrageenans from a single precursor carrying different protecting groups that can be cleaved specifically to introduce the sulfate groups at various positions depending on the targeted carrageenan.

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry
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Main Research Area: Technical/natural sciences
Electronic versions:
LIBRO_COMPLETO_EUROCARB4.pdf
Publication: Research - peer-review › Journal article – Annual report year: 2017

Transition Metal Catalyzed Synthesis of Carboxylic Acids, Imines, and Biaryls
Dehydrogenative synthesis of carboxylic acids catalyzed by a ruthenium N-heterocycliccarbene complex. A new methodology for the synthesis of carboxylic acids from primary alcohols and hydroxide has been developed. The reaction is catalyzed by the ruthenium N-heterocycliccarbene complex [RuCl4(IPr)(p-cymene)] where dihydrogen is generated as the only by-product (Scheme i). The dehydrogenative reaction is performed in toluene, which allows for a simple isolation of the products by precipitation followed by extraction. Various substituted benzyl alcohols smoothly undergo the
transformation. The fast conversion to the carboxylic acids can be explained by the involvement of a competing Cannizzaro reaction. The scope of the dehydrogenation was further extended to linear and branched saturated aliphatic alcohols, although longer reaction times are necessary to ensure complete substrate conversions. The kinetic isotope effect of the reaction was determined to be 0.67 using 1-butanol as the substrate. A plausible catalytic cycle was characterized by DFT/B3LYP-D3 and involved coordination of the alcohol to the metal, β-hydride elimination, hydroxide attack on the coordinated aldehyde, and a second β-hydride elimination to furnish the carboxylate. Mn catalyzed radical Kumada-type reaction between aryl halides and aryl Grignard reagents. The reaction between aryl halides and aryl Grignard reagents catalyzed by MnCl2 has been extended to several methyl-substituted aryl iodide reagents by hyperforming the reaction at 120 °C in a microwave oven (Scheme ii). A limitation of the heterocoupling process is the concomitant dehalogenation of the aryl halide and homocoupling of the Grignard reagent leading to moderate yields of the desired heterocoupling product. The mechanism of the cross-coupling process was investigated by performing two radical trap experiments. The employment of radical scavengers such as 1,4-cyclohexadiene and 4-(2-bromophenyl)but-1-ene revealed the presence of an aryl radical intermediate. This leads to the proposal of an SN1 pathway for the coupling.

Study of the dehydrogenative synthesis of imines from primary alcohols and amines catalyzed by manganese complexes. An initial study of the dehydrogenative synthesis of imines catalyzed by simple and commercially available manganese complexes has been conducted (Scheme iii). Originally the low valent CpMn(CO)3, Mn(CO)5Br, and Mn2(CO)10 complexes were employed for the coupling reaction between benzyl alcohol and cyclohexylamine, but these displayed only poor or no reactivity. Surprisingly when the Jacobsen complex is used as the catalyst, the reaction between benzyl alcohol and cyclohexylamine resulted in 77% yield of the corresponding imine. Moreover gas evolution confirmed that the reaction occurs by dehydrogenation.

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Organisations: Department of Chemistry, Organic Chemistry
Authors: Santilli, C. (Intern), Madsen, R. (Intern)
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Relations
Projects:

Transition Metal Catalyzed Synthesis of Carboxylic Acids, Imines, and Biaryls
Publication: Research › Ph.D. thesis – Annual report year: 2017

Trends in Strong Chemical Bonding in C2, CN, CN-, CO, N2, NO, NO+, and O2
The strong chemical bonds between C, N, and O play a central role in chemistry, and their formation and cleavage are critical steps in very many catalytic processes. The close-lying molecular orbital energies and large correlation effects pose a challenge to electronic structure calculations and have led to different bonding interpretations, most notably for C2. One way to approach this problem is by strict benchmark comparison of related systems. This work reports reference electronic structures and computed bond dissociation enthalpies D0 for C2, CN, CN-, CO, N2, NO, NO+, O2 and related systems C2+ and C2- at chemical accuracy (~1 kcal/mol or 4 kJ/mol) using CCSD(T)/aug-cc-pV5Z, with additional benchmarks of HF, MP2, CCSD, explicitly correlated F12 methods, and four density functionals. Very large correlation and basis set effects are responsible for up to 93% of total D0. The order of the molecular orbitals 1πu and 3σg changes, as seen in text books, depending on total and effective nuclear charge. Linear trends are observed in 20u - 20g orbital splitting (R2 = 0.91) and in D0 of C2, C2-, and C2+ (R2 = 0.99). The correlation component of D0 of C2 is by far the largest (~93%) due to a poor HF description. Importantly, density functional theory fails massively in describing this series consistently in both limits of effective nuclear charge, and Hartree-Fock-exchange or meta functionals do not remedy this 100 kJ/mol-error, which should thus be addressed in future density functional developments as it affects very many studies involving cleavage or formation of these bonds.

General information
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Organisations: Department of Chemistry
Authors: Kepp, K. P. (Intern)
Pages: 9092–9098
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Main Research Area: Technical/natural sciences
Two-dimensional nanomaterials supported electrochemical energy storage for smart grids
Ultra-broadband mid-wave-IR upconversion detection

In this Letter, we demonstrate efficient room temperature detection of ultra-broadband mid-wave-infrared (MWIR) light with an almost flat response over more than 1200 nm, exploiting an efficient nonlinear upconversion technique. Black-body radiation from a hot soldering iron rod is used as the IR test source. Placing a 20 mm long periodically poled lithium niobate crystal in a compact intra-cavity setup (> 20 WCW pump at 1064 nm), MWIR wavelengths ranging from 3.6 to 4.85 μm are upconverted to near-infrared (NIR) wavelengths (820-870 nm). The NIR light is detected using a standard low-noise silicon-based camera/grating spectrometer. The proposed technique allows high conversion efficiency over a wider bandwidth without any need for a shorter crystal length. Different analytical predictions and numerical simulations are performed a priori to support the experimental demonstrations. (C) 2017 Optical Society of America
Ultrafast X-ray absorption study of longitudinal-transverse phonon coupling in electrolyte aqueous solution

Ultrafast X-ray absorption spectroscopy is applied to study the conversion of longitudinal to transverse phonons in aqueous solution. Permanganate solutes serve as X-ray probe molecules that permit the measurement of the conversion of 13.5 GHz, longitudinal phonons to 27 GHz, transverse phonons that propagate with high-frequency sound speed. The experimental results, combined with QM/MM MD simulations, show that the hydrogen bond network around the charged solutes has a glass-like stiffness that persists for at least tens of picoseconds.
Ultralight, Flexible, and Semi-Transparent Metal Oxide Papers for Photoelectrochemical Water Splitting

Thanks to their versatile functionality, metal oxides (MOs) constitute one of the key family materials in a variety of current demands for sensor, catalysis, energy storage and conversion, optical electronics, and piezoelectric mechanics. Much effort has focused on engineering specific nanostructure and macroscopic morphology of MOs that aims to enhance their performances, but the design and controlled synthesis of ultrafine nanostructured MOs in a cost-effective and facile way remains a challenge. In this work, we have exploited the advantages of intrinsic structures of graphene oxide (GO) papers, serving as a sacrificial template, to design and synthesize two-dimensional (2D) layered and free-standing MO papers with ultrafine nanostructures. Physicochemical characterizations showed that these MO materials are nanostructured, porous, flexible, and ultralight. The as-synthesized materials were tested for their potential application in photoelectrochemical (PEC) energy conversion. In terms of PEC water splitting, copper oxide papers were used as an example and exhibited excellent performances with an extremely high photocurrent-to-weight ratio of 3 A cm⁻² g⁻¹. We have also shown that the synthesis method is generally valid for many earth-abundant transition metals including copper, nickel, iron, cobalt, and manganese.
Unexpected interactions between gold and N-morpholino-sulfonates

Nanoporous gold (NPG) has a high surface area and excellent conductivity. It is an ideal supporting material for the electrocatalysis, e.g. in fuel cell applications. NPG is traditionally produced by etching a gold/silver alloy. This method has significant drawbacks, such as the introduction of silver into your NPG, and its multi-step fabrication. A method has been discovered for producing NPG as a thin film chemically. This bottom-up approach entails reduction of Au3+ precursor using morpholinoethanesulfonic acid (MES). This produces a thin and highly porous gold film at the air-water interface1 (for details, see poster by Mikkel Christiansen). This chemical reaction is far more complex than first expected and by-products, intermediates and reaction mechanisms are the focus of the present work. The chemical reaction and its products have been examined using state-of-the-art nuclear magnetic resonance (NMR), ultraviolet-visible spectroscopy (UV-vis), fluorescence spectroscopy, density functional theory (DFT), mass spectrometry (MS) and Raman spectroscopy. The results illustrate a complex chain of reactions resulting in gold nanoparticles, NPG, and several previously unidentified Au-complexes. N-NMR presented three different 13+/+ environments for the N-atom in MES, while the UV-vis results points towards some interesting gold complexes. MS identifies several distinct molecular entities demonstrating the reactivity of MES and Au, and fluorescence spectroscopy suggests the formation of polynuclear Au complexes as previously reported where Au nuclei are bridged by C=N functionalities in small organic molecules 2. This adds up to a complicated reaction mechanism involving some interesting Au 3+/1+ complexes, deprotonation and oxidation of MES and the formation of molecules that show UV-vis absorbance and fluorescence.

General information

State: Published
Organisations: Department of Chemistry, NanoChemistry, Organic Chemistry, University of California, San Diego, University of Copenhagen
Authors: Nielsen, F. S. (Intern), Engelbrekt, C. (Intern), Elliot, S. G. (Intern), Junor, G. (Ekstern), Sørensen, K. (Ekstern), Jensen, K. J. (Ekstern), Clausen, M. H. (Intern), Zhang, J. (Intern)
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Source: PublicationPreSubmission
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Unified quantum theory of elastic and inelastic atomic scattering from a physisorbed monolayer solid

A unified quantum theory of the elastic and inelastic scattering of low energy He atoms by a physisorbed monolayer solid in the one-phonon approximation is given. It uses a time-dependent wave packet with phonon creation and annihilation components and has a self-consistent feedback between the wave functions for elastic and inelastic scattered atoms. An attenuation of diffraction scattering by inelastic processes thus is inherent in the theory. The atomic motion and monolayer vibrations in the harmonic approximation are treated quantum mechanically and unitarity is preserved. The evaluation of specific one-phonon events includes contributions from diffuse inelastic scattering in other phonon modes. Effects of thermally excited phonons are included using a mean field approximation. The theory is applied to an incommensurate Xe/Pt(111) monolayer (incident energy $E_i = 4$-16 meV), a commensurate Xe/graphite monolayer ($E_i$ similar or equal to 64 meV), and an incommensurate Xe/Cu(001) monolayer ($E_i$ similar or equal to 8 meV). The monolayers are very corrugated targets and there are transient closed diffraction and inelastic channels in the calculations. In many cases, the energy gain events have strengths comparable to the energy loss events.

General information
State: Published
Organisations: Department of Chemistry, Department of Applied Mathematics and Computer Science, Scientific Computing, University of Wisconsin-Madison
Authors: Bruch, L. W. (Ekstern), Hansen, F. Y. (Intern), Dammann, B. (Intern)
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Web of Science (2017): Indexed yes
Scopus rating (2016): CiteScore 3.16
Web of Science (2016): Indexed yes
Scopus rating (2015): SJR 1.933 SNIP 0.94 CiteScore 2.8
Web of Science (2015): Indexed yes
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Web of Science (2013): Indexed yes
Scopus rating (2012): SJR 3.206 SNIP 1.394 CiteScore 3.57
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
Scopus rating (2011): SJR 3.382 SNIP 1.438 CiteScore 3.61
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
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Web of Science (2010): Indexed yes
Scopus rating (2009): SJR 3.109 SNIP 1.474
Web of Science (2009): Indexed yes
Scopus rating (2008): SJR 2.982 SNIP 1.524
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 2.923 SNIP 1.546
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 2.796 SNIP 1.56
Whole grain-rich diet reduces body weight and systemic low-grade inflammation without inducing major changes of the gut microbiome: a randomised cross-over trial

Objective To investigate whether a whole grain diet alters the gut microbiome and insulin sensitivity, as well as biomarkers of metabolic health and gut functionality. Design 60 Danish adults at risk of developing metabolic syndrome were included in a randomised cross-over trial with two 8-week dietary intervention periods comprising whole grain diet and refined grain diet, separated by a washout period of ≥6 weeks. The response to the interventions on the gut microbiome composition and insulin sensitivity as well on measures of glucose and lipid metabolism, gut functionality, inflammatory markers, anthropometry and urine metabolomics were assessed. Results 50 participants completed both periods with a whole grain intake of 179±50 g/day and 13±10 g/day in the whole grain and refined grain period, respectively. Compliance was confirmed by a difference in plasma alkylresorcinols (p<0.0001). Compared with refined grain, whole grain did not significantly alter glucose homeostasis and did not induce major changes in the faecal microbiome. Also, breath hydrogen levels, plasma short-chain fatty acids, intestinal integrity and intestinal transit time were not affected. The whole grain diet did, however, compared with the refined grain diet, decrease body weight (p<0.0001), serum inflammatory markers, interleukin (IL)-6 (p=0.009) and C-reactive protein (p=0.003). The reduction in body weight was consistent with a reduction in energy intake, and IL-6 reduction was associated with the amount of whole grain consumed, in particular with intake of rye. Conclusion Compared with refined grain diet, whole grain diet did not alter insulin sensitivity and gut microbiome but reduced body weight and systemic low-grade inflammation.

General information
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Organisations: National Food Institute, Research Group for Gut Microbiology and Immunology, Department of Bio and Health Informatics, Metagenomics, Disease Intelligence and Molecular Evolution, Department of Biotechnology and Biomedicine, Disease Systems Immunology, Department of Chemical and Biochemical Engineering, Organic Chemistry, Center for BioProcess Engineering, DTU Multi Assay Core, Research Group for Analytical Food Chemistry, Copenhagen Center for Health Technology, University of Copenhagen, Chalmers University of Technology, Chalmers University of Technology, Bispebjerg University Hospital, Herlev and Gentofte Hospital, University of Auckland
Number of pages: 12
Publication date: 2017
Zeeman effect in sulfur monoxide: a tool to probe magnetic fields in star forming regions
Context. Magnetic fields play a fundamental role in star formation processes and the best method to evaluate their intensity is to measure the Zeeman effect of atomic and molecular lines. However, a direct measurement of the Zeeman spectral pattern from interstellar molecular species is challenging due to the high sensitivity and high spectral resolution required. So far, the Zeeman effect has been detected unambiguously in star forming regions for very few non-masing species, such as OH and CN. Aims. We decided to investigate the suitability of sulfur monoxide (SO), which is one of the
most abundant species in star forming regions, for probing the intensity of magnetic fields via the Zeeman effect. Methods. We investigated the Zeeman effect for several rotational transitions of SO in the (sub-)mm spectral regions by using a frequency-modulated, computer-controlled spectrometer, and by applying a magnetic field parallel to the radiation propagation (i.e., perpendicular to the oscillating magnetic field of the radiation). To support the experimental determination of the g factors of SO, a systematic quantum-chemical investigation of these parameters for both SO and O$_2$ has been carried out. Results. An effective experimental-computational strategy for providing accurate g factors as well as for identifying the rotational transitions showing the strongest Zeeman effect has been presented. Revised g factors have been obtained from a large number of SO rotational transitions between 86 and 389 GHz. In particular, the rotational transitions showing the largest Zeeman shifts are: N,J = 2, 2 ← 1, 1 (86.1 GHz), N,J = 4, 3 ← 3, 2 (159.0 GHz), N,J = 1, 1 ← 0, 1 (286.3 GHz), N,J = 2, 2 ← 1, 2 (309.5 GHz), and N,J = 2, 1 ← 1, 0 (329.4 GHz). Our investigation supports SO as a good candidate for probing magnetic fields in high-density star forming regions.

General information
State: Published
Organisations: Department of Chemistry, Università di Bologna, University of Mainz, INAF, Osservatorio Astronomico di Arcetri, Instituto de CC. de Materiales de Madrid (ICMM-CSIC), Instituto de Astrofísica de Canarias
Authors: Cazzoli, G. (Ekstern), Lattanzi, V. (Ekstern), Coriani, S. (Intern), Gauss, J. (Ekstern), Codella, C. (Ekstern), Ramos, A. A. (Ekstern), Cernicharo, J. (Ekstern), Puzzarini, C. (Ekstern)
Publication date: 2017
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Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 2.543 SNIP 1.189 CiteScore 3.5
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.823 SNIP 1.219 CiteScore 2.82
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.544 SNIP 1.058 CiteScore 2.01
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 2.585 SNIP 1.295 CiteScore 3.14
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 2.373 SNIP 1.231 CiteScore 3.42
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 2.74 SNIP 1.444
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.879 SNIP 1.404
Web of Science (2009): Indexed yes
Graphene-polymer-enzyme hybrid nanomaterials for biosensors
The invention relates to a general chemical method for the synthesis of biocompatible hybrid nanomaterials which can be used in the development of new-type enzyme based biosensors. A one-step facile method is presented, in which polyethylenimine (PEI) serves as both a reducing agent for the reduction of graphene oxide (GO) into reduced graphene oxide (RGO) and a biological matrix for accommodation of enzymes.

General information
State: Published
Organisations: Department of Chemistry, NanoChemistry, Organic Chemistry
Authors: Chi, Q. (Intern), Han, S. (Intern), Halder, A. (Intern), Zhu, N. (Intern), Ulstrup, J. (Intern)
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Priority number: EP20140195093
Original language: English
Main Research Area: Technical/natural sciences
Source: espacenet
Source-ID: WO2016083204
Publication: Research - Patent – Annual report year: 2016
Process for reducing the oxygen content of biomass using molybdenum-based catalysts
The present invention concerns a process for converting biomass into useful organic building blocks for the chemical
industry. The process involves the reduction of a polyol wherein at least two of the hydroxyl groups are located on
adjacent carbon atoms in the presence of a molybdenum-based catalyst of the formula (I), such as (NH$_4$)$_6$Mo$_7$O$_{24}$-4H$_2$O.
A primary or secondary monohydric C1-C4 alcohol is used as reductant, as well as a solvent.

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry
Authors: Dethlefsen, J. R. (Intern), Fristrup, P. (Intern)
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Source: espacenet
Source-ID: WO2016078673
Publication: Research › Patent – Annual report year: 2016

119Sn MAS NMR Study of Probe Molecules Interaction with Sn-BEA: The Origin of Penta- and Hexacoordinated Tin
Formation
$^{119}$Sn CPMG MAS NMR was applied to study the adsorption of acetonitrile, methanol, isopropanol, isobutanol and water
over Sn-BEA enriched with $^{119}$Sn isotope. Two signals observed at ca. -422 and -443 ppm over dehydrated samples
were attributed to tetracoordinated framework tin sites with strong and weak Lewis acidity, respectively. The adsorption of
acetonitrile and methanol resulted in observation of pentacoordinated tin species, due to the formation of 1:1 adsorption
complexes over both Sn-sites. Water adsorption led first to formation of pentacoordinated tin species, which were further
converted into hexacoordinated species at longer reaction times. The latter transformation was found to be kinetically
limited and was attributed to chemical interaction of tin sites with water, such as hydrolysis of Si-O-Sn bonds. The
adsorption of isopropanol and isobutanol was accompanied by the formation of pentacoordinated Sn species in the case
of weak sites and hexacoordinated Sn over sites with strong Lewis acidity, pointing to the possibility of dissociative
adsorption of secondary alcohols over strong Sn-sites.

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry, Moscow Lomonosov State University, Moscow State
University, Haldor Topsoe AS
Authors: Yakimov, A. V. (Ekstern), G. Kolyagin, Y. (Ekstern), Tolborg, S. (Intern), Vennestrøm, P. N. R. (Ekstern),
Ivanova, I. I. (Ekstern)
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Scopus rating (2016): CiteScore 4.48 SJR 1.948 SNIP 1.181
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Absorption and oxidation of nitrogen oxide in ionic liquids

A new strategy for capturing nitrogen oxide, NO, from the gas phase is presented. Dilute NO gas is removed from the gas phase by ionic liquids under ambient conditions. The nitrate anion of the ionic liquid catalyzes the oxidation of NO to nitric acid by atmospheric oxygen in the presence of water. The nitric acid is absorbed in the ionic liquid up to approximately one mole HNO₃ per mole of the ionic liquid due to the formation of hydrogen bonds. The nitric acid can be desorbed by heating, thereby regenerating the ionic liquid with excellent reproducibility. Here, time-resolved in-situ spectroscopic investigations of the reaction and products are presented. The procedure reveals a new vision for removing the pollutant NO by absorption into a non-volatile liquid and converting it into a useful bulk chemical, that is, HNO₃.

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry, Centre for Catalysis and Sustainable Chemistry
Accelerated synthesis of Sn-BEA in fluoride media: effect of H2O content in the gel

Tin-containing zeotypes, particularly Sn-BEA, are promising heterogeneous catalysts for a number of important industrially relevant reactions. However, the direct hydrothermal synthesis of these materials requires unfavourably long times, which is an obstacle for their industrial application. In the present study we show that up to 4-fold reduction of the crystallization time can be achieved by the decreasing of the H2O/SiO2 ratio in the synthesis gel from 7.5 to 5.6. The crystallization kinetics has been studied for five series of gels containing 1.0 SiO2: 0.27 TEA2O : x SnO2 : 0.54 HF : y H2O, for which y was fixed to 5.6, 6.8 and 7.7 at x = 0.005 and to 5.6 and 6.8 at x = 0.010. The crystallization time was varied within 0.5 – 60 days. The intermediate and final products obtained were investigated using XRD, FTIR, XRF, SEM, UV-Vis, MAS NMR spectroscopy and nitrogen adsorption-desorption techniques. The products obtained with lower water content are shown to have the same structure, textural properties and morphology as materials synthesized with higher water content. Although the size of the crystals is found to decrease with water content in the gel, it does not affect the Sn coordination and environment as confirmed by 119Sn MAS NMR.

General information

State: Published
Organisations: Department of Chemistry, Organic Chemistry, Moscow Lomonosov State University, Haldor Topsoe AS
Authors: Yakimov, A. V. (Ekstern), Kolyagin, Y. G. (Ekstern), Tolborg, S. (Intern), Vennestrøm, P. N. R. (Ekstern), Ivanova, I. I. (Ekstern)
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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
Accessing Tri-substituted γ-Lactam Scaffolds Via Cascade Reactions: What Opportunities For Libraries!

The European Lead Factory is an EU-based initiative (part of the Innovative Medicines Initiative), which has been set to foster drug discovery in Europe. Among the objectives, a 200,000-compound collection is being generated. Lactams represent a large class of valuable scaffolds for medicinal chemistry and remain a wide and interesting area of study. In this context, 2 libraries based on a 1,4,5 γ-lactam core have been designed and produced using cascade reactions involving an aldehyde moiety, an amine and a nucleophilic partner as the key reaction. One library is focused on a 3-MCR on oxo-esters, while the other is based on a Ritter-type cascade. On several occasions these multi-component and one-pot processes have been used directly as the production step, thus allowing very fast and diverse library syntheses, whereas in other cases, the choice of partners bearing other anchoring groups permitted further functionalization and the production of even more diverse members of the libraries. The > 1,000 compounds based on these scaffolds have been delivered for HTS at the European Screening Center where they are currently being tested.

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry, Department of Organic Chemistry, EDELRIS
Authors: Bonnet, K. (Ekstern), Clausen, M. H. (Intern), Fleury-Brégeot, N. (Ekstern), Lardy, C. (Ekstern), Morgentin, R. (Ekstern), Nielsen, T. E. (Intern), Petersen, M. A. (Intern), Rasmussen, M. O. (Ekstern), Roche, D. (Ekstern), Wu, P. (Intern)
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Main Research Area: Technical/natural sciences
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http://www.fasebj.org/content/30/1_Supplement/lb473.abstract
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Acetaldehyde as an Intermediate in the Electroreduction of Carbon Monoxide to Ethanol on Oxide-Derived Copper

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

General information
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ISI indexed (2012): ISI indexed no
Web of Science (2012): Indexed yes
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BFI (2010): BFI-level 1
BFI (2009): BFI-level 1
BFI (2008): BFI-level 1
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Electronic versions:
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Acetaldehyde as an Intermediate in the Electroreduction of Carbon Monoxide to Ethanol on Oxide-Derived Copper

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

General information

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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
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Scopus rating (2013): SJR 5.681 SNIP 2.204 CiteScore 10.7
ISI indexed (2013): ISI indexed yes
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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
Acetate production enhancement from carbon dioxide reduction by using modified cathode materials in microbial electrosynthesis

Microbial electrosynthesis (MES) is one of the emerging biosustainable technologies for the biological conversion of carbon dioxide to the value-added chemical precursor. The electro autotrophic bacteria fix CO₂ via Wood-Ljungdahl pathway, accepting the electron derived from the cathode in the bioelectrochemical System (BES). The MES reactor can power with the solar photovoltaic system and harvest light energy to multi-carbon compounds to make it artificial photosynthesis system. Nevertheless, chemical production rate should be optimized for the commercialization of MES technology. Interestingly, it has been demonstrated that the productivity was enhanced with the modified cathode surfaces by improving microbe-electrode electron transfer. Here, we have tested the different cathode materials for the improvement of acetate production from carbon dioxide and their behavior for the biofilm formation. Interestingly, graphene based electrode materials has better performance on the acetate production and microbe-electrode interaction. Modification with three dimensional metal-graphene networks increased the electrosynthesis rate of acetate from CO₂ by 10.2 fold compared with three-dimensional graphene network by using sporomusa ovata.

General information
State: Published
Organisations: Novo Nordisk Foundation Center for Biosustainability, Research Groups, Department of Chemistry, NanoChemistry, Organic Chemistry
Authors: Aryal, N. (Intern), Halder, A. (Intern), Zhang, M. (Intern), Tremblay, P. (Intern), Chi, Q. (Intern), Zhang, T. (Intern)
Number of pages: 1
Acid-Base Bifunctional Zirconium N-Alkyltriphosphate Nanohybrid for Hydrogen Transfer of Biomass-Derived Carboxides

Catalytic transfer hydrogenation (CTH) reactions are efficient transformation routes to upgrade biobased chemicals. Herein, we report a facile and template-free route to synthesize a series of heterogeneous nitrogen-containing alkyltriphosphonate-metal hybrids with enhancing Lewis acid and base sites, and their catalytic activity in converting biomass-derived carbonyl compounds to corresponding alcohols in 2-propanol. Particularly, a quantitative yield of furfuryl alcohol (FFA) was obtained from furfural (FUR) over organotriphosphate-zirconium hybrid (ZrPN) under mild conditions. The presence of Lewis basic sites adjacent to acid sites with an appropriate base/acid site ratio (1:0.7) in ZrPN significantly improved the yield of FFA. Mechanistic studies for the transformation of FUR to FFA with ZrPN in 2-propanol-d8 evidently indicate CTH reaction proceeding via a direct intermolecular hydrogen transfer route. It was also found that ZrPN could catalyze isomerization of C-3-C-6 aldoses to ketoses involving intramolecular hydrogen transfer in water.
A Correlation between the Activity of Candida antarctica Lipase B and Differences in Binding Free Energies of Organic Solvent and Substrate

The ability of enzymes to operate in organic solvent is now widely accepted and is the basis for extensive research in enzymology. The challenge is to select the solvent media that allows the modulation of enzyme activity. For a rational selection of a solvent, it is necessary to understand the effect of organic solvent molecules on enzyme structure and the enzymatic reaction on a molecular level. To gain such insight, we combined experimental kinetics studies with full atomic molecular dynamics simulations and found a correlation between the activity of Candida antarctica lipase B (CALB) [for the esterification reaction between butyric acid and ethanol at a fixed water activity] and the binding of the solvent/substrate molecules in the active site region of CALB. We have investigated the influence of four organic solvents hexane (HEX), methyl tertiary butyl ether (MTBE), acetonitrile (ACN), and tertiary butanol (TBU)-on the catalytic activity of CALB for the esterification reaction. The solvents have been chosen on the basis of different polarity/functional groups. Our study shows that these organic solvents do not alter the overall conformation of CALB; rather, the solvent effects on the performance of the enzyme may be ascribed to binding of solvent molecules to the enzyme active site region and the solvation energy of substrate molecules in the different solvents. Polar solvent molecules interact strongly with CALB and compete with the substrate to bind to the active site region, resulting in an inhibitory effect which is also confirmed by the binding free energies for the solvent and substrate molecules estimated from the simulations. Consequently, the catalytic activity of CALB decreases in polar solvents. This effect is significant, and CALB is over 10 orders of magnitude more active in nonpolar solvents (HEX and MTBE) than in the polar solvents (ACN and TBU). TBU molecules show an exceptional behavior because the solvent molecule forms an extensive hydrogen bond network within the CALB active site region suggesting that solvent molecules rich on hydrogen bond acceptors and donors are poor solvents when used for lipase-catalyzed esterification reactions.
Advanced purification strategy for CueR, a cysteine containing copper(I) and DNA binding protein

Metal ion regulation is essential for living organisms. In prokaryotes metal ion dependent transcriptional factors, the so-called metalloregulatory proteins play a fundamental role in controlling the concentration of metal ions. These proteins recognize metal ions with an outstanding selectivity. A detailed understanding of their function may be exploited in potential health, environmental and analytical applications. Members of the MerR protein family sense a broad range of mostly late transition and heavy metal ions through their cysteine thiolates. The air sensitivity of latter groups makes the expression and purification of such proteins challenging. Here we describe a method for the purification of the copper-regulatory CueR protein under optimized conditions. In order to avoid protein precipitation and/or eventual aggregation and to get rid of the co-purifying Escherichia coli elongation factor, our procedure consisted of four steps supplemented by DNA digestion. Subsequent anion exchange on Sepharose FF Q 16/10, affinity chromatography on Heparin FF 16/10, second anion exchange on Source 30 Q 16/13 and gel filtration on Superdex 75 26/60 resulted in large amounts of pure CueR protein without any affinity tag. Structure and functionality tests performed with mass spectrometry, circular dichroism spectroscopy and electrophoretic gel mobility shift assays approved the success of the purification procedure.
Affinity Induced Surface Functionalization of Liposomes Using Cu-Free Click Chemistry

Functionalization of nanoparticles is a key element for improving specificity of drug delivery systems toward diseased tissue or cells. In the current study we report a highly efficient and chemoselective method for post-functionalization of liposomes with biomacromolecules, which equally well can be used for functionalization of other nanoparticles or solid surfaces. The method exploits a synergistic effect of having both affinity and covalent anchoring tags on the surface of the liposome. This was achieved by synthesizing a peptide linker system that uses Cu-free strain-promoted click chemistry in combination with histidine affinity tags. The investigation of post-functionalization of PEGylated liposomes was performed with a cyclic RGDfE peptide. By exploring both affinity and covalent tags a 98 ± 2.0% coupling efficiency was achieved, even a diluted system showed a coupling efficiency of 87 ± 0.2%. The reaction kinetics and overall yield were quantified by HPLC. The results presented here open new possibilities for constructing complex nanostructures and functionalized surfaces.
Algal toxicity of platinum nanoparticles - Implications of NP aggregation, dissolution and shading

General information
State: Published
Organisations: Department of Environmental Engineering, Environmental Chemistry, Department of Chemistry, NanoChemistry, Organic Chemistry, Department of Micro- and Nanotechnology, Nano Bio Integrated Systems, University of Geneva, Technical University of Denmark
Authors: Sørensen, S. N. (Intern), Engelbrekt, C. (Intern), Lützhøft, H. H. (Intern), Jiménez-Lamana, J. (Ekstern), Noori, J. S. (Intern), Giron Delgado, C. (Ekstern), Slaveykova, V. (Ekstern), Baun, A. (Intern)
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Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2016

Alternative NOx abatement, finding a suitable method
This project explores the possibility of removing NOx through one of several strategies utilising the unique properties of ionic liquids (ILs), including absorption and oxidation of NOx to nitric acid.

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry
Authors: Jakobsen, P. W. (Intern), Mossin, S. (Intern), Fehrmann, R. (Intern)
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Main Research Area: Technical/natural sciences
Links:
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Sustain Abstract E-7
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2016

Alzheimer's disease due to loss of function: A new synthesis of the available data
Alzheimer's Disease (AD) is a highly complex disease involving a broad range of clinical, cellular, and biochemical manifestations that are currently not understood in combination. This has led to many views of AD, e.g. the amyloid, tau, presenilin, oxidative stress, and metal hypotheses. The amyloid hypothesis has dominated the field with its assumption that buildup of pathogenic β-amyloid (Aβ) peptide causes disease. This paradigm has been criticized, yet most data suggest that Aβ plays a key role in the disease. Here, a new loss-of-function hypothesis is synthesized that accounts for the anomalies of the amyloid hypothesis, e.g. the curious pathogenicity of the Aβ42/Aβ40 ratio, the loss of Aβ caused by presenilin mutation, the mixed phenotypes of APP mutations, the poor clinical-biochemical correlations for genetic variant carriers, and the failure of Aβ reducing drugs. The amyloid-loss view accounts for recent findings on the structure and chemical features of Aβ variants and their coupling to human patient data. The lost normal function of APP/Aβ is argued to be metal transport across neuronal membranes, a view with no apparent anomalies and substantially more explanatory power than the gain-of-function amyloid hypothesis. In the loss-of-function scenario, the central event of Aβ aggregation is interpreted as a loss of soluble, functional monomer Aβ, rather than toxic overload of oligomers. Accordingly, new research models and treatment strategies should focus on remediation of the functional amyloid balance, rather than strict containment of Aβ, which, for reasons rationalized in this review, has failed clinically.

General information
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Organisations: Department of Chemistry
A metal-catalyzed enyne-cyclization step for the synthesis of bi- and tricyclic scaffolds amenable to molecular library production

A facile metal-catalyzed diversification step for the synthesis of novel bi- and tricyclic scaffolds from enyne substrates is reported in this study. From a single starting material, topologically diverse scaffolds for library synthesis can be generated and decorated in a few steps. The methodology was used to produce a library of 490 compounds within the European Lead Factory (ELF) Consortium.
A Mouse Positron Emission Tomography Study of the Biodistribution of Gold Nanoparticles with Different Surface Coatings Using Embedded Copper-64

By taking advantage of the ability of (64)Cu to bind non-specifically to gold surfaces, we have developed a new methodology to embed this radionuclide inside gold nanoparticles (AuNPs). (64)Cu enables the in vivo imaging of AuNPs by positron emission tomography (PET). AuNPs have a multitude of uses within health technology and are useful tools for general nanoparticle research. (64)Cu-AuNPs were prepared by incubating AuNP seeds with (64)Cu(2+), followed by the entrapment of the radionuclide by grafting a second layer of gold on the surface. This resulted in radiolabeling efficiencies of 53 ± 6%. The radiolabel showed excellent stability when challenging with EDTA for two days (>95% radioactivity retention) and showed no loss of (64)Cu when incubated with 50% mouse serum for two days. The methodology was chelator-free, and circumvents traditional concerns over chelator instability and altered AuNP properties due to surface modification. Radiolabeled (64)Cu-AuNP cores were prepared in a biomedically relevant size of 30 nm and used to investigate the in vivo stability of three different AuNP coatings by PET imaging in a murine xenograft tumor model. We found the longest plasma half-life (T½ = 9 hours) and highest tumor accumulation (3.9 %ID/g) by using polyethylene glycol (PEG) coating, while faster elimination from the bloodstream was observed with both a Tween 20-stabilized coating and a zwitterionic coating based on a mixture of sulfonic acids and quaternary amines, which has previously been reported to be superior to PEG. The new embedding method provides the utilization of PET imaging in combination with the multitude of uses that AuNPs have found in health technology, and the method can equally well be utilized for therapeutic copper radioisotopes for use in radiotherapy.

General information
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Organisations: Department of Micro- and Nanotechnology, Department of Electrical Engineering, Colloids and Biological Interfaces, Center for Nuclear Technologies, The Hevesy Laboratory, Department of Chemistry, University of Copenhagen
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 13.65 SJR 6.916 SNIP 2.65
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
A Multimethod Approach for Investigating Algal Toxicity of Platinum Nanoparticles

The ecotoxicity of platinum nanoparticles (PtNPs) widely used in for example automotive catalytic converters, is largely unknown. This study employs various characterization techniques and toxicity end points to investigate PtNP toxicity toward the green microalgae Pseudokirchneriella subcapitata and Chlamydomonas reinhardtii. Growth rate inhibition occurred in standard ISO tests (EC\text{50} values of 15–200 mg Pt/L), but also in a double-vial setup, separating cells from PtNPs, thus demonstrating shading as an important artifact for PtNP toxicity. Negligible membrane damage, but substantial oxidative stress was detected at 0.1–80 mg Pt/L in both algal species using flow cytometry. PtNPs caused growth rate inhibition and oxidative stress in P. subcapitata, beyond what was accounted for by dissolved Pt, indicating NP-specific toxicity of PtNPs. Overall, P. subcapitata was found to be more sensitive toward PtNPs and higher body burdens were measured in this species, possibly due to a favored binding of Pt to the polysaccharide-rich cell wall of this algal species. This study highlights the importance of using multimethod approaches in nanoecotoxicological studies to elucidate toxicity mechanisms, influence of NP-interactions with media/organisms, and ultimately to identify artifacts and appropriate end points for NP-ecotoxicity testing.

General information

State: Published
Organisations: Department of Environmental Engineering, Environmental Chemistry, Department of Chemistry, NanoChemistry, Organic Chemistry, Infection Microbiology, Department of Micro- and Nanotechnology, University of Geneva, IPM-Intelligent Pollutant Monitoring, Technical University of Denmark
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Journal: Environmental Science and Technology
Volume: 50
Issue number: 19
ISSN (Print): 0013-936X
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BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
An ATP Binding Cassette Transporter Mediates the Uptake of α-(1,6)-Linked Dietary Oligosaccharides in *Bifidobacterium* and Correlates with Competitive Growth on These Substrates

The molecular details and impact of oligosaccharide uptake by distinct human gut microbiota (HGM) are currently not well understood. Non-digestible dietary galacto- and gluco-(1,6)-oligosaccharides from legumes and starch, respectively, are preferentially fermented by mainly bifidobacteria and lactobacilli in the human gut. Here we show that the solute binding protein (BlG16BP) associated with an ATP binding cassette (ABC) transporter from the probiotic *Bifidobacterium animalis* subsp. *lactis* Bl-04 binds -(1,6)-linked glucosides and galactosides of varying size, linkage, and monosaccharide composition with preference for the trisaccharides raffinose and panose. This preference is also reflected in the -(1,6)-galactoside uptake profile of the bacterium. Structures of BlG16BP in complex with raffinose and panose revealed the basis for the remarkable ligand binding plasticity of BlG16BP, which recognizes the non-reducing -(1,6)-diglycoside in its ligands. BlG16BP homologues occur predominantly in bifidobacteria and a few Firmicutes but lack in other HGMs. Among seven bifidobacterial taxa, only those possessing this transporter displayed growth on -(1,6)-glycosides. Competition assays revealed that the dominant HGM commensal *Bacteroides* ovatus was out-competed by *B. animalis* subsp. *lactis* Bl-04 in mixed cultures growing on raffinose, the preferred ligand for the BlG16BP. By comparison, *B. ovatus* monocultures grew very efficiently on this trisaccharide. These findings suggest that the ABC-mediated uptake of raffinose provides an important competitive advantage, particularly against dominant *Bacteroides* that lack glycan-specific ABC-transporters. This novel insight highlights the role of glycan transport in defining the metabolic specialization of gut bacteria.

General information
State: Published
Organisations: Department of Systems Biology, Enzyme and Protein Chemistry, Department of Chemistry, Department of Micro- and Nanotechnology, Colloids and Biological Interfaces, Lund University, University of Groningen
Authors: Hansen, M. E. (Intern), Fredslund, F. (Ekstern), Andersen, J. M. (Intern), Žagar, A. V. (Ekstern), Henriksen, J. R. (Intern), Andresen, T. L. (Intern), Svensson, B. (Intern), Slotboom, D. J. (Ekstern), Abou Hachem, M. (Intern)
Number of pages: 12
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Publication date: 2016
Main Research Area: Technical/natural sciences

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Volume: 291
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Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.17 SJR 2.755 SNIP 1.125
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 3.121 SNIP 1.184 CiteScore 4.4
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 3.254 SNIP 1.222 CiteScore 4.5
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 3.369 SNIP 1.231 CiteScore 4.87
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 3.361 SNIP 1.244 CiteScore 4.97
ISI indexed (2012): ISI indexed yes
An efficient arabinoxylan-debranching α-l-arabinofuranosidase of family GH62 from Aspergillus nidulans contains a secondary carbohydrate binding site

An α-l-arabinofuranosidase of family GH62 from Aspergillus nidulans FGSC A4 (AnAbf62A-m2,3) has an unusually high activity towards wheat arabinoxylan (WAX) (67 U/mg; $k_{cat} = 178$/s, $K_m = 4.90$ mg/ml) and arabinoxylooligosaccharides (AXOS) with degrees of polymerisation (DP) 3–5 (37–80 U/mg), but about 50 times lower activity for sugar beet arabinan and 4-nitrophenyl-α-l-arabinofuranoside. α-1,2- and α-1,3-linked arabinofuranoses are released from monosubstituted, but not from disubstituted, xylose in WAX and different AXOS as demonstrated by NMR and polysaccharide analysis by carbohydrate gel electrophoresis (PACE). Mutants of the predicted general acid (Glu188) and base (Asp28) catalysts, and the general acid pKa modulator (Asp136) lost 1700-, 165- and 130-fold activities for WAX. WAX, oat spelt xylan, birchwood xylan and barley β-glucan retarded migration of AnAbf62A-m2,3 in affinity electrophoresis (AE) although the latter two are neither substrates nor inhibitors. Trp23 and Tyr44, situated about 30 Å from the catalytic site as seen in an AnAbf62A-m2,3 homology model generated using Streptomyces thermoviolaceus SthAbf62A as template, participate in...
carbohydrate binding. Compared to wild-type, W23A and W23A/Y44A mutants are less retarded in AE, maintain about 70% activity towards WAX with K_i of WAX substrate inhibition increasing 4–7-folds, but lost 77–96% activity for the AXOS. The Y44A single mutant had less effect, suggesting Trp^{23} is a key determinant. AnAbf62A-m2,3 seems to apply different polysaccharide-dependent binding modes, and Trp^{23} and Tyr^{44} belong to a putative surface binding site which is situated at a distance of the active site and has to be occupied to achieve full activity.

**General information**
State: Published
Organisations: Department of Systems Biology, Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, Enzyme and Protein Chemistry, Department of Chemistry, Metalloprotein Chemistry and Engineering, Organic Chemistry, Carlsberg Laboratory, University of Cambridge, University of Copenhagen, Megazyme International Ireland Ltd.
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.57 SJR 1.177 SNIP 1.173
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.254 SNIP 1.217 CiteScore 3.43
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.327 SNIP 1.458 CiteScore 3.71
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.533 SNIP 1.432 CiteScore 4.3
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.507 SNIP 1.286 CiteScore 4
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.437 SNIP 1.232 CiteScore 3.72
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.381 SNIP 1.239
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.353 SNIP 1.062
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
119Sn CPMG MAS NMR is demonstrated to be a fast and efficient method for characterization of Sn-sites in Sn-containing zeolites. Tuning of the CPMG echo-train sequence decreases the experimental time by a factor of 5–40 in the case of as-synthesized and hydrated Sn-BEA samples and by 3 orders of magnitude in the case of dehydrated Sn-BEA samples as compared to conventional methods. In the latter case, the reconstruction of the quantitative spectrum without the loss of sensitivity is shown to be possible. The method proposed allows obtaining 119Sn MAS NMR spectra with improved resolution for Sn-BEA zeolites with natural 119Sn isotope abundance using conventional MAS NMR equipment.
A Quantitative Scale of Oxophilicity and Thiophilicity

Oxophilicity and thiophilicity are widely used concepts with no quantitative definition. In this paper, a simple, generic scale is developed that solves issues with reference states and system dependencies and captures empirically known tendencies toward oxygen. This enables a detailed analysis of the fundamental causes of oxophilicity. Notably, the notion that oxophilicity relates to Lewis acid hardness is invalid. Rather, oxophilicity correlates only modestly and inversely with absolute hardness and more strongly with electronegativity and effective nuclear charge. Since oxygen is highly electronegative, ionic bonding is stronger to metals of low electronegativity. Left-side d-block elements with low effective nuclear charges and electro-negativities are thus highly oxophilic, and the f-block elements, not because of their hardness, which is normal, but as a result of the small ionization energies of their outermost valence electrons, can easily transfer electrons to fulfill the electron demands of oxygen. Consistent with empirical experience, the most oxophilic elements are found in the left part of the d block, the lanthanides, and the actinides. The d-block elements differ substantially in oxophilicity, quantifying their different uses in a wide range of chemical reactions; thus, the use of mixed oxo- and thiophilic (i.e., "mesophilic") surfaces and catalysts as a design principle can explain the success of many recent applications. The proposed scale may therefore help to rationalize and improve chemical reactions more effectively than current qualitative considerations of oxophilicity.
Main Research Area: Technical/natural sciences

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BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.64 SJR 1.774 SNIP 1.198
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.805 SNIP 1.239 CiteScore 4.7
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.869 SNIP 1.314 CiteScore 4.69
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.819 SNIP 1.379 CiteScore 4.9
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 2.08 SNIP 1.35 CiteScore 4.72
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.952 SNIP 1.373 CiteScore 4.64
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.98 SNIP 1.323
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.982 SNIP 1.47
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 2.025 SNIP 1.412
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 2.136 SNIP 1.544
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.828 SNIP 1.508
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 2.012 SNIP 1.46
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.672 SNIP 1.382
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.498 SNIP 1.465
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 1.616 SNIP 1.398
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 1.749 SNIP 1.511
We present a facile synthesis protocol for atomically thin platinum (Pt) shells on top of gold (Au) nanoparticles (NPs) (Au@PtNPs) in one pot under mild conditions. The Au@PtNPs exhibited remarkable stability (> 2 years) at room temperature. The synthesis, bimetallic nanostructures and catalytic properties were thoroughly characterized by ultraviolet-visible light spectrophotometry, transmission electron microscopy, nanoparticle tracking analysis and electrochemistry. The 8 ± 2 nm Au@PtNPs contained 24 ± 1 mol% Pt and 76 ± 1 mol% Au corresponding to an atomically thin Pt shell. Electrochemical data clearly show that the active surface is dominated by Pt with a specific surface area above 45 m² per gram of Pt. Interactions with the Au core increase the activity of the Pt shell by up to 55% and improve catalytic selectivity compared to pure Pt. The Au@Pt NPs show exciting catalytic activity in electrooxidation of sustainable fuels (i.e. formic acid, methanol and ethanol), and selective hydrogenation of benzene derivatives. Especially high activity was achieved for formic acid oxidation, 549 mA (mgPt)−1 (at 0.6 V vs. SCE), which is 3.5 fold higher than a commercial < 5 nm PtNP catalyst. Excellent activity for the direct production of γ-valerolactone, an alternative biofuel/fuel additive, from levulinic acid and methyl levulinate was finally demonstrated.

**General information**

State: Published
Organisations: Department of Chemistry, NanoChemistry, Organic Chemistry, Centre for Catalysis and Sustainable Chemistry
Authors: Engelbrekt, C. (Intern), Seselj, N. (Intern), Poreddy, R. (Intern), Riisager, A. (Intern), Ulstrup, J. (Intern), Zhang, J. (Intern)
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  - Scopus rating (2016): CiteScore 8.46 SJR 3.037 SNIP 1.468
  - Web of Science (2016): Indexed yes
  - BFI (2015): BFI-level 1
  - Scopus rating (2015): SJR 2.672 SNIP 1.663 CiteScore 8.36
  - Web of Science (2015): Indexed yes
  - BFI (2014): BFI-level 1
  - Scopus rating (2014): SJR 2.343 SNIP 1.526 CiteScore 7.27
  - Web of Science (2014): Indexed yes
  - BFI (2013): BFI-level 1
  - ISI indexed (2013): ISI indexed no
  - Web of Science (2013): Indexed yes
Original language: English
Electronic versions: c5ta08922k.pdf
Atomistic characterization of the active-site solvation dynamics of a model photocatalyst

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

Liposomes for medical applications are often administered by intravenous injection. Once in the bloodstream, the liposomes are covered with a "protein corona", which impacts the behavior and eventual fate of the liposomes. Currently, many aspects of the liposomal protein corona are not well understood. For example, there is generally a lack of knowledge about the liposome binding affinities and dynamics of common types of blood plasma proteins. Fluorescence correlation spectroscopy (FCS) is a powerful experimental technique that potentially can provide such knowledge. In this study, we have used FCS to investigate the binding of human serum albumin (HSA) to standard types of PEGylated fluid-phase liposomes (consisting of DOPC and DOPE-PEG2k) and PEGylated gel-phase liposomes (consisting of DSPC and DSPE-PEG2k) with various PEG chain surface densities. We detected no significant binding of HSA to the PEGylated fluid-phase liposomes. In contrast, we found that HSA bound tightly to the PEGylated gel-phase liposomes, although only a low number of HSA molecules could be accommodated per liposome. Overall, we believe that our data provides a useful benchmark for other researchers interested in studying the liposomal protein corona.

General information
State: Published
Organisations: Department of Micro- and Nanotechnology, Colloids and Biological Interfaces, Department of Chemistry
Authors: Kristensen, K. (Intern), Urquhart, A. (Intern), Thor mann, E. (Intern), Andresen, T. L. (Intern)
Publication date: 2016
Event: Poster session presented at The 43rd Annual Meeting & Exposition of the Controlled Release Society, Seattle, WA, United States.
Main Research Area: Technical/natural sciences
Electronic versions:
Poster_Kasper_Kristensen.pdf
Source: PublicationPreSubmission
Source-ID: 127758941
Publication: Research - peer-review › Poster – Annual report year: 2016

Binding of human serum albumin to PEGylated liposomes: insights into binding numbers and dynamics by fluorescence correlation spectroscopy

Liposomes for medical applications are often administered by intravenous injection. Once in the bloodstream, the liposomes are covered with a "protein corona", which impacts the behavior and eventual fate of the liposomes. Currently, many aspects of the liposomal protein corona are not well understood. For example, there is generally a lack of knowledge about the liposome binding affinities and dynamics of common types of blood plasma proteins. Fluorescence correlation spectroscopy (FCS) is a powerful experimental technique that potentially can provide such knowledge. In this study, we have used FCS to investigate the binding of human serum albumin (HSA) to standard types of PEGylated fluid-phase liposomes (consisting of DOPC and DOPE-PEG2k) and PEGylated gel-phase liposomes (consisting of DSPC and DSPE-PEG2k) with various PEG chain surface densities. We detected no significant binding of HSA to the PEGylated fluid-phase liposomes. In contrast, we found that HSA bound tightly to the PEGylated gel-phase liposomes, although only a low number of HSA molecules could be accommodated per liposome. Overall, we believe that our data provides a useful benchmark for other researchers interested in studying the liposomal protein corona.

General information
State: Published
Organisations: Department of Micro- and Nanotechnology, Colloids and Biological Interfaces, Department of Chemistry
Authors: Kristensen, K. (Intern), Urquhart, A. (Intern), Thor mann, E. (Intern), Andresen, T. L. (Intern)
Number of pages: 11
Pages: 19726-19736
Publication date: 2016
Main Research Area: Technical/natural sciences
Bioengineering of Solution Processed Graphene for the Development of Ultrasensitive Flexible Biosensing Platform

Development of low-cost, flexible and ultrasensitive biosensing platforms for rapid detection of different human metabolites is of great importance for the healthcare, pharmaceuticals and biomedical diagnostics sectors. Synthesis of novel functionalized nanomaterials with high surface area is a key step in the fabrication of high flexible biosensing devices. Flexible biosensors are one of the most promising next generation wearable self-monitoring devices, as material flexibility is very crucial to attach on a patient’s body part and maintaining the mechanical stability as well as the sensing responses. In recent years, graphene based materials have invoked a new era for developing smart hybrid material based biosensors. Graphene could offer a perfect solution as an ideal signal transducer for the development of low-cost bioelectronics devices.

General information
State: Published
Organisations: Department of Chemistry, NanoChemistry, Organic Chemistry, Department of Micro- and Nanotechnology
Authors: Halder, A. (Intern), Hemanth, S. (Intern), Keller, S. S. (Intern), Ulstrup, J. (Intern), Chi, Q. (Intern)
Publication date: 2016
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Publication information
Journal: Electrochemical Society. Meeting Abstracts (Online)
Volume: MA2016-02
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Black perithecial pigmentation in *Fusarium* species is due to the accumulation of 5-deoxybostrycoidin-based melanin

Biosynthesis of the black perithecial pigment in the filamentous fungus *Fusarium graminearum* is dependent on the polyketide synthase PGL1 (oPKS3). A seven-membered PGL1 gene cluster was identified by over-expression of the cluster specific transcription factor pglR. Targeted gene replacement showed that PGL1, pglJ, pglM and pglV were essential for the production of the perithecial pigment. Over-expression of PGL1 resulted in the production of 6-O-demethyl-5-deoxybostrycoidin (1), 5-deoxybostrycoidin (2), and three novel compounds 5-deoxybostrycoidin anthrone (3), 6-O-demethyl-5-deoxybostrycoidin anthrone (4) and purpurfusarin (5). The novel dimeric bostrycoidin purpurfusarin (5) was found to inhibit the growth of *Candida albicans* with an IC50 of 8.0 +/-1.9 μM. The results show that *Fusarium* species with black perithecia have a previously undescribed form of 5-deoxybostrycoidin based melanin in their fruiting bodies.

General information

State: Published

Organisations: Department of Systems Biology, Eucaryotic Molecular Cell Biology, Department of Chemistry, Organic Chemistry, Norwegian Veterinary Institute, University of Oslo, Norwegian Institute of Bioeconomy Research, Aalborg University


Number of pages: 13

Publication date: 2016

Main Research Area: Technical/natural sciences

Publication information

Journal: Scientific Reports

Volume: 6

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BFI (2018): BFI-level 1

Web of Science (2018): Indexed yes

BFI (2017): BFI-level 1

Web of Science (2017): Indexed yes

BFI (2016): BFI-level 1

Scopus rating (2016): CiteScore 4.63 SJR 1.625 SNIP 1.401

Web of Science (2016): Indexed yes

BFI (2015): BFI-level 1

Scopus rating (2015): SJR 2.057 SNIP 1.684 CiteScore 5.3

Web of Science (2015): Indexed yes

BFI (2014): BFI-level 1

Scopus rating (2014): SJR 2.103 SNIP 1.544 CiteScore 4.75

Web of Science (2014): Indexed yes

BFI (2013): BFI-level 1

Scopus rating (2013): SJR 1.886 SNIP 1.51 CiteScore 4.06

ISI indexed (2013): ISI indexed yes

Web of Science (2013): Indexed yes

BFI (2012): BFI-level 1

Scopus rating (2012): SJR 1.458 SNIP 0.896 CiteScore 2.44

ISI indexed (2012): ISI indexed yes

Web of Science (2012): Indexed yes

ISI indexed (2011): ISI indexed no

Original language: English

Fungal biology, Metabolomics, Molecular evolution

Electronic versions:

Black_perithecial_pigmentation_in_Fusarium_species_is_due_to_the_accumulation_of_5_deoxybostrycoidin_based_melanin.pdf
Brønsted Acid Ionic Liquids (BAILs) as Efficient and Recyclable Catalysts in the Conversion of Glycerol to Solketal at Room Temperature

Brønsted acid ionic liquids (BAILs) have been prepared and applied for the first time - to the best of our knowledge - as efficient catalysts in the acetylation of glycerol with acetone to form solketal ((2,2-dimethyl-1,3-dioxolan-4-yl)methanol) at very mild reaction conditions (room temperature) and short reaction times. The BAILs showed a superior catalytic performance in terms of both conversion and selectivity compared to the common mineral acid methanesulfonic acid as well as to other reported homogeneous and heterogeneous catalysts. Catalyst reusability was demonstrated with one of the BAILs (BAIL-1), which was recovered and reused by a simple procedure in four consecutive reaction runs without any loss of catalytic activity and selectivity. Thus, the BAILs combine the advantages of both homogeneous and heterogeneous catalysis with respect to excellent conversion and selectivity as well as easy recyclability.

Butterfly Deformation Modes in a Photoexcited Pyrazolate-Bridged Pt Complex Measured by Time-Resolved X-Ray Scattering in Solution

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

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Department of Chemistry, Northwestern University, Argonne National Laboratory, North Carolina State University
Number of pages: 9
Pages: 7475-7483
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Physical Chemistry A
Volume: 120
Issue number: 38
ISSN (Print): 1089-5639
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.64
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 2.78
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 2.65
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 2.84
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 2.78
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 2.87
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Web of Science (2008): Indexed yes
Web of Science (2007): Indexed yes
Web of Science (2006): Indexed yes
Web of Science (2005): Indexed yes
Web of Science (2004): Indexed yes
Catalytic Enantioselective Synthesis of Tetrahydocarbazoles and Exocyclic Pictet-Spengler-Type Reactions

A synthetic strategy for the synthesis of chiral tetrahydrocarbazoles (THCAs) has been developed. The strategy relies on two types of 6-exo-trig cyclization of 3-substituted indole substrates. Enantioselective domino Friedel-Crafts-type reactions leading to THCAs can be catalyzed by chiral phosphoric acid derivatives (with up to >99% ee), and the first examples of exocyclic Pictet-Spengler reactions to form THCAs are reported.

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry
Number of pages: 4
Pages: 5990-5993
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Organic Letters
Volume: 18
Issue number: 23
ISSN (Print): 1523-7060
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 6.32 SJR 2.964 SNIP 1.218
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 3.055 SNIP 1.336 CiteScore 6.38
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.958 SNIP 1.324 CiteScore 6.18
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 3.144 SNIP 1.329 CiteScore 6.12
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 3.312 SNIP 1.355 CiteScore 5.7
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 3.271 SNIP 1.377 CiteScore 5.81
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 2
Characterization of the LM5 pectic galactan epitope with synthetic analogues of β-1,4-d-galactotetraose

Plant cell wall glycans are important polymers that are crucial to plant development and serve as an important source of sustainable biomass. The study of polysaccharides in the plant cell wall relies heavily on monoclonal antibodies for localization and visualization of glycans, using e.g. Immunofluorescent microscopy. Here, we describe the detailed epitope mapping of the mab LM5 that is shown to bind to a minimum of three sugar residues at the non-reducing end of linear beta-1,4-linked galactan. The study uses de novo synthetic analogs of galactans combined with carbohydrate microarray and competitive inhibition ELISA for analysis of antibody-carbohydrate interactions.

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry, University of Leeds, University of Copenhagen
Authors: Andersen, M. C. F. (Intern), Boos, I. (Intern), Marcus, S. E. (Ekstern), Kračun, S. K. (Ekstern), Rydahl, M. G. (Ekstern), Willats, W. G. (Ekstern), Knox, J. P. (Ekstern), Clausen, M. H. (Intern)
Pages: 36–40
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Carbohydrate Research
Volume: 436
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BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Characterizing the Solvated Structure of Photoexcited \([\text{Os(terpy)}_2]^{2+}\) with X-ray Transient Absorption Spectroscopy and DFT Calculations

Characterizing the geometric and electronic structures of individual photoexcited dye molecules in solution is an important step towards understanding the interfacial properties of photo-active electrodes. The broad family of "red sensitizers" based on osmium(II) polypyridyl compounds often undergoes small photo-induced structural changes which are challenging to characterize. In this work, X-ray transient absorption spectroscopy with picosecond temporal resolution is
employed to determine the geometric and electronic structures of the photoexcited triplet state of \([\text{Os(terpy)}_2]^{2+}\) (terpy: 2,2':6',2″-terpyridine) solvated in methanol. From the EXAFS analysis, the structural changes can be characterized by a slight overall expansion of the first coordination shell \([\text{OsN}_6]\). DFT calculations supports the XTA results. They also provide additional information about the nature of the molecular orbitals that contribute to the optical spectrum (with TD-DFT) and the near-edge region of the X-ray spectra.

**General information**
State: Published
Organisations: Department of Chemistry, Tianjin Polytechnical University, Deutsches Elektronen-Synchrotron, Argonne National Laboratory
Authors: Zhang, X. (Ekstern), Pápai, M. I. (Intern), Møller, K. B. (Intern), Zhang, J. (Ekstern), Canton, S. E. (Ekstern)
Number of pages: 9
Publication date: 2016
Main Research Area: Technical/natural sciences

**Publication information**
Journal: Molecules
Volume: 21
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ISSN (Print): 1420-3049
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BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.09 SJR 0.809 SNIP 1.231
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.562 SNIP 1.168 CiteScore 2.65
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.725 SNIP 1.31 CiteScore 2.62
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.707 SNIP 1.283 CiteScore 2.61
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.791 SNIP 1.365 CiteScore 2.87
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.723 SNIP 1.138 CiteScore 2.54
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.561 SNIP 1.14
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.524 SNIP 1.016
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.425 SNIP 0.764
Scopus rating (2007): SJR 0.399 SNIP 0.849
Scopus rating (2006): SJR 0.388 SNIP 0.762
Scopus rating (2005): SJR 0.455 SNIP 0.718
Scopus rating (2004): SJR 0.286 SNIP 0.475
Chemical Synthesis of Hemicellulose Fragments

Hemicelluloses constitute a significant part of plant biomass, yet so far it has been difficult to make use of this class of polysaccharides. A lack of access to this class of molecules prevents the use of enzymatic studies to increase our understanding of the biochemical processes relevant to the synthesis and degradation of hemicellulose. In this thesis the synthesis of arabinoxylans as well as glucuronoxylans is demonstrated. At first, a reliable strategy to efficiently synthesize a variety of xylan backbones was established. Two strategies were tried. The first strategy was an attempt to use an unprotected xylose acceptor in a tin-mediated glycosylation. Since the best results of the optimization of this reaction were not good enough a second strategy was pursued. This second strategy is based on the preactivation of thioglycosides to be glycosylated with thioglycoside acceptors which in turn can be preactivated again in a second step. Optimization of this strategy lead to a viable pathway towards a variety of protected xylan backbones. The use of protecting groups allows for the specific introduction of branching units to the backbone. Subsequently arabinose as well as glucuronic acid were attached to the xylan backbone.

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry
Authors: Böhm, M. F. (Intern), Madsen, R. (Intern)
Number of pages: 140
Publication date: 2016

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

Relations
Projects:
Chemical Synthesis of Hemicellulose Fragments
Source: PublicationPreSubmission
Source-ID: 127352926
Publication: Research › Ph.D. thesis – Annual report year: 2016

Chemodiversity of Ladder-Frame Prymnesin Polyethers in Prymnesium parvum
Blooms of the microalga Prymnesium parvum cause devastating fish kills worldwide, which are suspected to be caused by the supersized ladder-frame polyether toxins prymnesin-1 and -2. These toxins have, however, only been detected from P. parvum in rare cases since they were originally described two decades ago. Here, we report the isolation and characterization of a novel B-type prymnesin, based on extensive analysis of 2D- and 3D-NMR data of natural as well as 90% 13C enriched material. B-type prymnesins lack a complete 1,6-dioxadecalin core unit, which is replaced by a short acyclic C2 linkage compared to the structure of the original prymnesins. Comparison of the bioactivity of prymnesin-2 with prymnesin-B1 in an RTgill-W1 cell line assay identified both compounds as toxic in the low nanomolar range. Chemical investigations by liquid chromatography highresolution mass spectrometry (LC-HRMS) of 10 strains of P. parvum collected

Chemical Synthesis of Hemicellulose Fragments

Chemosynthesis of Hemicellulose Fragments

Chemosynthesis of Hemicellulose Fragments

Chemosynthesis of Hemicellulose Fragments
worldwide showed that only one strain produced the original prymnesin-1 and -2, whereas four strains produced the novel B-type prymnesin. In total 13 further prymnesin analogues differing in their core backbone and chlorination and glycosylation patterns could be tentatively detected by LC-MS/HRMS, including a likely C-type prymnesin in five strains. Altogether, our work indicates that evolution of prymnesins has yielded a diverse family of fish-killing toxins that occurs around the globe and has significant ecological and economic impact.

General information
State: Published
Organisations: Department of Systems Biology, Department of Chemistry, Organic Chemistry, Metabolomics Platform, University of Copenhagen
Authors: Rasmussen, S. A. (Intern), Meier, S. (Intern), Andersen, N. G. (Ekstern), Blossom, H. E. (Ekstern), Duus, J. Ø. (Intern), Nielsen, K. F. (Intern), Hansen, P. J. (Ekstern), Larsen, T. O. (Intern)
Number of pages: 7
Pages: 2250-2256
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Main Research Area: Technical/natural sciences

Publication information
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BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.41 SJR 1.22 SNIP 1.408
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.395 SNIP 1.758 CiteScore 4.14
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.333 SNIP 1.827 CiteScore 3.68
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.516 SNIP 1.716 CiteScore 3.75
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.428 SNIP 1.538 CiteScore 3.23
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.39 SNIP 1.508 CiteScore 3.11
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.368 SNIP 1.601
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.461 SNIP 1.5
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.328 SNIP 1.423
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.248 SNIP 1.505
Web of Science (2007): Indexed yes
Chemodiversity of the ladder-frame prymnesin polyethers of the fish-killing microalgal Prymnesium parvum

General information
State: Published
Organisations: Department of Systems Biology, Department of Chemistry, Organic Chemistry, Metabolomics Platform, University of Copenhagen
Authors: Rasmussen, S. A. (Intern), Meier, S. (Intern), Gedsted Andersen, N. (Ekstern), Blossom, H. (Ekstern), Duus, J. Ø. (Intern), Nielsen, K. F. (Intern), Larsen, T. O. (Intern)
Number of pages: 1
Publication date: 2016
Conference: 9th Joint Meeting of AFERP, ASP, GA, JSP, PSE & SIF, Copenhagen, Denmark, 24/07/2016 - 24/07/2016
Main Research Area: Technical/natural sciences

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Volume: 81
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Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.97 SJR 0.654 SNIP 0.94
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.637 SNIP 0.991 CiteScore 2.1
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.762 SNIP 1.135 CiteScore 2.15
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.789 SNIP 1.246 CiteScore 2.37
Chemoselective hydrogenation of arenes by PVP supported Rh nanoparticles

Polyvinylpyrrolidone-stabilized Rh nanoparticles (RhNPs/PVP) of ca. 2.2 nm in size were prepared by the hydrogenation of the organometallic complex \([\text{Rh}(\eta^3-\text{C}_3\text{H}_5)_3]\) in the presence of PVP and evaluated as a catalyst in the hydrogenation of a series of arene substrates as well as levulinic acid and methyl levulinate. The catalyst showed excellent activity and selectivity towards aromatic ring hydrogenation compared to other reported transition metal-based catalysts under mild reaction conditions (room temperature and 1 bar \(\text{H}_2\)). Furthermore, it was shown to be a highly promising catalyst for the hydrogenation of levulinic acid and methyl levulinate in water leading to quantitative formation of the fuel additive \(\gamma\)-valerolactone under moderate reaction conditions compared to previously reported catalytic systems.

General information

State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry, CNRS, Universite de Toulouse
Authors: Ibrahim, M. (Ekstern), Poreddy, R. (Intern), Philippot, K. (Ekstern), Riisager, A. (Intern), Garcia-Suarez, E. J. (Intern)
Number of pages: 6
Pages: 19368-19373
Publication date: 2016
Main Research Area: Technical/natural sciences
BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.85 SJR 1.243 SNIP 0.931
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.351 SNIP 1.026 CiteScore 4.1
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.413 SNIP 1.085 CiteScore 4.06
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.436 SNIP 1.083 CiteScore 4.07
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.554 SNIP 1.001 CiteScore 3.79
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.505 SNIP 1.013 CiteScore 3.68
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.399 SNIP 0.875
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.928 SNIP 0.783
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.629 SNIP 0.572
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.669 SNIP 0.539
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.084 SNIP 0.907
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.128 SNIP 0.815
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.045 SNIP 0.933
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.1 SNIP 1.051
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 0.973 SNIP 0.827
Scopus rating (2001): SJR 0.626 SNIP 0.488
Scopus rating (2000): SJR 0.318 SNIP 0.183
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 0.29 SNIP 0.188
Original language: English
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Chemoselective_hydrogenation.pdf
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10.1039/C6DT03668F
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Chiral Selectivity in Inter-reactant Recognition and Electron Transfer of the Oxidation of Horse Heart Cytochrome c by Trioxalatocobaltate(III)

We have studied electron transfer between cytochrome c and the chiral transition-metal complex pair Λ- and Δ-[Co(Ox)₃]³⁻ (Ox²⁻ = oxalate) via strong ion-pair formation. Chirality was found in both ion-pair formation and electron transfer, with the Λ enantiomer the more strongly bound and faster reacting. Investigations of the chirality using electron-transfer theory combined with quantum-chemical and statistical-mechanical calculations showed that chirality is solely in inter-reactant interaction and electronic overlap.

General information
State: Published
Organisations: Department of Chemistry, NanoChemistry, Organic Chemistry, Kazan National Research Technological University, Technical University of Denmark
Authors: Nazmutdinov, R. R. (Ekstern), Bronshtein, M. D. (Ekstern), Zinkicheva, T. T. (Ekstern), Hansen, N. S. (Ekstern), Zhang, J. (Intern), Ulstrup, J. (Intern)
Number of pages: 11
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Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.64 SJR 1.774 SNIP 1.198
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.805 SNIP 1.239 CiteScore 4.7
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.869 SNIP 1.314 CiteScore 4.69
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.819 SNIP 1.379 CiteScore 4.9
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 2.08 SNIP 1.35 CiteScore 4.72
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.952 SNIP 1.373 CiteScore 4.64
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.98 SNIP 1.323
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.982 SNIP 1.47
Web of Science (2009): Indexed yes
Co-assembly of chitosan and phospholipids into hybrid hydrogels

Novel hybrid hydrogels were formed by adding chitosan (Ch) to phospholipids (P) self-assembled particles in lactic acid. The effect of the phospholipid concentration on the hydrogel properties was investigated and was observed to affect the rate of hydrogel formation and viscoelastic properties. A lower concentration of phospholipids (0.5% wt/v) in the mixture, facilitates faster network formation as observed by Dynamic Light Scattering, with lower elastic modulus than the hydrogels formed with higher phospholipid content. The nano-porous structure of Ch/P hydrogels, with a diameter of 260±20 nm, as observed by cryo-scanning electron microscopy, facilitated the penetration of water and swelling. Cell studies revealed suitable biocompatibility of the Ch/P hydrogels that can be used within life sciences applications.

General information
State: Published
Authors: Mendes, A. C. L. (Intern), Shekarforoush, E. (Intern), Engwer, C. (Ekstern), Beeren, S. (Intern), Goycoolea, F. M. (Ekstern), Chronakis, I. S. (Intern)
Pages: 905-916
Publication date: 2016
Conference: 12th Conference of the European Chitin Society, Münster, Germany, 30/08/2016 - 30/08/2016
Main Research Area: Technical/natural sciences
Combined Function of Brønsted and Lewis Acidity in the Zeolite-Catalyzed Isomerization of Glucose to Fructose in Alcohols

Glucose conversion via fructose to useful chemicals and fuels has attracted considerable attention. Isomerization of glucose to fructose can proceed along several different reaction pathways involving different sugar intermediates and isomeric forms. Presently, the roles of the substrate isomeric forms and of the catalyst properties remain incompletely understood. By using NMR spectroscopy, we elucidate the interplay of the catalyst active sites in converting monosaccharide forms to products, byproducts, and intermediates in alcohols.
Composite nanomaterials of semiconductors and noble metals as plasmonic photocatalysts

Harnessing sunlight and storing the energy in chemical bonds is an important element in the transition towards green and sustainable technologies. Solar fuel production requires photocatalysts that (1) absorb large parts of the solar spectrum, (2) generate charges with significant lifetimes and appropriate energies, (3) catalyze relevant chemical transformations from abundant, low-energy starting materials, and (4) are stable under operating conditions. A new avenue within solar fuels involves plasmonic metal nanoparticles (PNPs). These materials have tunable optical properties, exciting catalytic behavior, and can be more stable under operating conditions. Composite photocatalysts of semiconductor nanoparticles (SNPs) and PNPs exploit broadly the solar spectrum, provide new catalytic routes and expand the scope of solar photocatalysis. The newly initiated project aims at developing composite nanomaterials of SNPs and PNPs from mild, aqueous synthesis protocols and testing the catalytic properties of these plasmonic photocatalysts.

General information
State: Published
Organisations: Department of Chemistry, NanoChemistry, Organic Chemistry, University of California
Authors: Engelbrekt, C. (Intern), Law, M. (Ekstern), Zhang, J. (Intern)
Number of pages: 1
Publication date: 2016
Event: Poster session presented at International Conference on Advances in Semiconductors and Catalysts for Photoelectrochemical Fuel Production (SolarFuel16), Berlin, Germany.
Main Research Area: Technical/natural sciences
Electronic versions: 2016.09_SolarFuels16_v3.pdf
Composition-dependent variation of magnetic properties and interstitial ordering in homogeneous expanded austenite

The crystal structure and magnetic properties of austenitic stainless steel with a colossal interstitial content, so-called expanded austenite, are currently not completely understood. In the present work, the magnetic properties of homogeneous samples of expanded austenite, as prepared by lowerature nitriding of thin foils, were investigated with magnetometry and Mössbauer spectroscopy. At room temperature, expanded austenite is paramagnetic for relatively low and for relatively high nitrogen contents ($y_N = 0.13$ and $0.55$, respectively, where $y_N$ is the interstitial nitrogen occupancy), while ferromagnetism is observed for intermediate nitrogen loads. Spontaneous volume magnetostriction was observed in the ferromagnetic state and the Curie temperature was found to depend strongly on the nitrogen content. For the first time, X-ray diffraction evidence for the occurrence of long-range interstitial order of nitrogen atoms in expanded austenite was observed for high nitrogen contents.
Constructing three-dimensional quasi-vertical nanosheet architectures from self-assemble two-dimensional WO$_3$·2H$_2$O for efficient electrochromic devices

Three-dimensional (3D) quasi-vertical nanosheet (QVNS) architectures are of great importance in the application of electrochromic devices due to its 3D porous structures, large surface area and lamellar permeable space of nanosheets. In this study, we demonstrate successful preparing of WO$_3$·2H$_2$O nanosheets via a novel and facile solution route and repurposing the typical electrodeposition technique to obtain 3D QVNS electrodes. The electrode was successfully assembled into an electrochromic device which exhibits good electrochromic performance.

General information
State: Published
Organisations: Department of Chemistry, NanoChemistry, Department of Chemistry, Organic Chemistry, Donghua University, Shanghai Second Polytechnic University
Authors: Li, H. (Ekstern), Wang, J. (Ekstern), Shi, Q. (Ekstern), Zhang, M. (Intern), Hou, C. (Intern), Shi, G. (Ekstern), Wang, H. (Intern), Zhang, Q. (Ekstern), Li, Y. (Ekstern), Chi, Q. (Intern)
Number of pages: 7
Pages: 281-287
Publication date: 2016
Conference: 10th International Conference on Surfaces, Coatings and Nanostructured Materials (NANOSMAT-10), Manchester, United Kingdom, 13/09/2015 - 13/09/2015
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BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.37 SJR 0.951 SNIP 1.225
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.914 SNIP 1.3 CiteScore 3.13
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.958 SNIP 1.477 CiteScore 2.96
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.965 SNIP 1.488 CiteScore 2.78
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.918 SNIP 1.373 CiteScore 2.26
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.908 SNIP 1.402 CiteScore 2.27
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.924 SNIP 1.141
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.842 SNIP 1.023
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.899 SNIP 1.087
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.795 SNIP 0.945
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 0.852 SNIP 1.052
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.679 SNIP 0.946
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.964 SNIP 1.126
Scopus rating (2003): SJR 0.988 SNIP 1.027
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 0.921 SNIP 0.954
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.841 SNIP 0.796
Scopus rating (2000): SJR 0.866 SNIP 0.772
Scopus rating (1999): SJR 1.064 SNIP 0.907
Original language: English
3D architectures, WO3·2H2O nanosheets, Electrodeposition, Electrochromic devices
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Construction of Insulin 18-mer Nanoassemblies Driven by Coordination to Iron(II) and Zinc(II) Ions at Distinct Sites

Controlled self-assembly (SA) of proteins offers the possibility to tune their properties or to create new materials. Herein, we present the synthesis of a modified human insulin (HI) with two distinct metal-ion binding sites, one native, the other abiotic, enabling hierarchical SA through coordination with two different metal ions. Selective attachment of an abiotic 2,2’-bipyridine (bipy) ligand to HI, yielding HI–bipy, enabled Zn(II)-binding hexamers to SA into trimers of hexamers, \([\text{HI–bipy}]_6^3\), driven by octahedral coordination to a Fe(II) ion. The structures were studied in solution by small-angle X-ray scattering and on surfaces with AFM. The abiotic metal ligand had a higher affinity for Fe(II) than Zn(II) ions, enabling control of the hexamer formation with Zn(II) and the formation of trimers of hexamers with Fe(II) ions. This precise control of protein SA to give oligomers of oligomers provides nanoscale structures with potential applications in nanomedicine.

General information
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BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
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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
Construction of Insulin 18-mer Nanoassemblies Driven by Coordination to Iron(II) and Zinc(II) Ions at Distinct Sites

Controlled self-assembly (SA) of proteins offers the possibility to tune their properties or to create new materials. Herein, we present the synthesis of a modified human insulin (HI) with two distinct metal-ion binding sites, one native, the other abiotic, enabling hierarchical SA through coordination with two different metal ions. Selective attachment of an abiotic 2,2’-bipyridine (bipy) ligand to HI, yielding HI–bipy, enabled ZnII-binding hexamers to SA into trimers of hexamers, [HI–bipy]$_6^3$, driven by octahedral coordination to a FeII ion. The structures were studied in solution by small-angle X-ray scattering and on surfaces with AFM. The abiotic metal ligand had a higher affinity for FeII than ZnII ions, enabling control of the hexamer formation with ZnII and the formation of trimers of hexamers with FeII ions. This precise control of protein SA to give oligomers of oligomers provides nanoscale structures with potential applications in nanomedicine.

General information

State: Published
Organisations: Department of Chemistry, NanoChemistry, Organic Chemistry, University of Copenhagen, Lund University, Novo Nordisk A/S
Number of pages: 4
Pages: 2424-2427
Publication date: 2016
Main Research Area: Technical/natural sciences

General information
State: Published
Organisations: Center for Atomic-scale Materials Design, Department of Chemistry, Department of Physics, Neutrons and X-rays for Materials Physics
Authors: Dohn, A. O. (Intern), Biasin, E. (Intern), Haldrup, K. (Intern), Nielsen, M. M. (Intern), Henriksen, N. E. (Intern), Møller, K. B. (Intern)
Number of pages: 1
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Physics B: Atomic, Molecular and Optical Physics
Volume: 49
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Article number: 059501
ISSN (Print): 0953-4075
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 1.22 SJR 0.616 SNIP 0.541
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.791 SNIP 0.806 CiteScore 1.19
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.121 SNIP 0.905 CiteScore 1.5
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.089 SNIP 0.943 CiteScore 1.62
CO₂ capture. Two new structures in the 2-amino-2-methyl-1-propanol (AMP) – water – CO₂ system

Energy production and transportation is responsible for more than 60 % of our CO₂ emission. In particular coal-fired power plants are big contributors. However, these large scale facilities offer the possibility to effective CO₂ capture through post-combustion processes. There are several options for such CO₂ capture. The problem is to make the absorption/desorption processes energetically and thereby economically viable. One process under investigation involves alkanoamines as absorbents in aqueous solutions. In these systems CO₂ is captured either by carbonate and/orcarbamate formation. We have studied the 2-amino-2-methyl-1-propanol (AMP) and the AMP-water phase diagramand its ability for CO₂ capture. The first crystal structure in the AMP – water system has been solved from powder diffraction data: AMP trihydrate (triclinic, P-1, a = 6.5897(3), b = 6.399 (2), c = 6.3399(2) Å and α = 92.40 (3), β =113.345(3) and γ = 94. 06(2) °). In the AMP – water CO₂ system two structures, a carbamate, AMPH-AMPCO₂ and a carbonate, (AMPH)₂-CO₃ are known [1]. In this work we solved a new structure from powder diffraction data, AMPH-HCO₃ hydrate (monoclinic, I2/a, a = 21.8522( ), b = 6.2149(15), c = 12.1300(3) Å, β = 104.036(16) °) readily formedwhen using <40 at% AMP in water.

General information
State: Published
Organisations: Department of Chemistry, X-ray Crystallography, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Ressources Engineering
Authors: Ståhl, K. (Intern), Neerup, R. (Intern), Fosbøl, P. L. (Intern)
Pages: 94-95
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Host publication information
Title of host publication: The European Power Diffraction Conference (EPDIC15) - Book of Abstracts
Crown-Ether Derived Graphene Hybrid Composite for Membrane-Free Potentiometric Sensing of Alkali Metal Ions

We report the design and synthesis of newly functionalized graphene hybrid material that can be used for selective membrane-free potentiometric detection of alkali metal ions, represented by potassium ions. Reduced graphene oxide (RGO) functionalized covalently by 18-crown[6] ether with a dense surface coverage is achieved by the introduction of a flexible linking molecule. The resulting hybrid composite is highly stable and is capable of detecting potassium ions down to micromolar ranges with a selectivity over other cations (including Ca^{2+}, Li^+, Na^+, NH_4^+) at concentrations up to 25 mM. This material can be combined further with disposable chips, demonstrating its promise as an effective ion-selective sensing component for practical applications.
Primary congenital glaucoma (PCG OMIM 231300) can be caused by pathogenic sequence variations in cytochrome P450, subfamily 1, polypeptide 1 (CYP1B1). The purpose of this study was to investigate the contribution of sequence variations in CYP1B1 in a cohort of individuals with PCG residing in Denmark. The study included 37 unrelated individuals with PCG. Individuals were investigated for CYP1B1 mutations by Sanger sequencing of polymerase chain reaction products using BigDye terminators and capillary electrophoresis. A total of 12 mutations were identified and 5 of these were novel. Six were missense mutations; 4 were truncating mutations (2 nonsense and 2 frameshift); 1 was an in-frame deletion and 1 was an in-frame duplication. Mutations in CYP1B1 could fully explain the PCG phenotype in 7 individuals (18%). Five individuals were compound heterozygous or presumed compound heterozygous, 1 was homozygous and 1 was apparently homozygous. Three individuals were heterozygous for sequence variations in CYP1B1 thought to be pathogenic—one of these was p.(Tyr81Asn). Several known sequence variations with presumably no functional effect were found in the cohort. In this study, we identified 12 CYP1B1 mutations, 5 of which were novel. The frequency of CYP1B1 mutations in this cohort was comparable with other populations. We also detected an individual heterozygous for p.(Tyr81Asn) mutation, previously suggested to cause autosomal dominant primary open-angle glaucoma.
Dehydrogenative Synthesis of Carboxylic Acids from Primary Alcohols and Hydroxide Catalyzed by a Ruthenium N-Heterocyclic Carbene Complex

Primary alcohols have been reacted with hydroxide and the ruthenium complex [RuCl2(IIPr)(p-cymene)] to afford carboxylic acids and dihydrogen. The dehydrogenative reaction is performed in toluene, which allows for a simple isolation of the products by precipitation and extraction. The transformation can be applied to a range of benzylic and saturated aliphatic alcohols containing halide and (thio)ether substituents, while olefins and ester groups are not compatible with the reaction conditions. Benzylic alcohols undergo faster conversion than other substrates, and a competing Cannizzaro reaction is most likely involved in this case. The kinetic isotope effect was determined to be 0.67 using 1-butanol as the substrate. A plausible catalytic cycle was characterized by DFT/B3LYP-D3 and involved coordination of the alcohol to the metal, β-hydride elimination, hydroxide attack on the coordinated aldehyde, and a second β-hydride elimination to furnish the carboxylate.
Densities of the binary system methane + n-decane have been determined through a vibrating tube densitometer from (278.15-463.15) K at pressures up to 140 MPa, and for methane mole fractions up to 0.8496. Negative excess volumes were found under the experimental conditions studied. Moreover isothermal compressibility values were obtained by differentiation from the Tammann-Tait correlation of the determined density values. Isobaric thermal expansion coefficients were also calculated based on differentiation from the isobaric fit of density data. We also measured the phase equilibrium of this binary system by using a variable volume cell with full visibility from (293.15-472.47) K for three mixtures with methane mole fractions of 0.4031, 0.6021 and 0.8496. Liquid fraction upon expansion below the saturation pressure has also been determined. Finally different equations of state were used to calculate the experimental density and excess...
volume data as well as the phase envelope data. No direct regression of the experimental data was involved in most of the
calculation in order to provide a fair comparison of the performance of different models.
Deprotonation of g-C$_3$N$_4$ with Na ions for efficient nonsacrificial water splitting under visible light

Developing a photocatalyst with the necessary characteristics of being cheap, efficient and robust for visible-light-driven water splitting remains a serious challenge within the photocatalysis field. Herein, an effective strategy, deprotonating g-C$_3$N$_4$ with Na ions from low-cost precursors, is reported. The deprotonated g-C3N4 exhibits a stable and reproducible H$_2$ and O$_2$ evolution rate of 31.5 and 15.2 μmol h$^{-1}$ from pure water over 24 h. Our findings reveal that the extraordinary photoreactivity comes from the enhanced optical absorption, the promoted charge transfer, and the completely inhibited H$_2$O$_2$ intermediate due to the deprotonation.
Design of porous nanostructured solid catalysts
This thesis aims at developing and characterize novel porous nanostructured materials for heterogeneous catalysis. The catalysts are prepared with the goals of increased activity and stability in mind. This will result in lessened waste of precious elements, starting materials, and energy, for a more sustainable chemical industry. Chapter 1 gives a short introduction to the effect of heterogeneous catalysis upon the current chemical industry. The scope of the thesis will also be sketched. Chapter 2 is a description of the methods used in the thesis, to characterize the materials produced. These include X-ray powder diffraction, physisorption analysis, and electron microscopy. This include common use, and possible pitfalls. Chapter 3 is an introduction to zeolites and their properties, mainly shape selectivity and catalytic activity. The diffusion limitations imposed by the porous system in zeolites will be examined as well, and strategies on how to overcome these limitations will be presented. Chapter 4 describes the synthesis of mesoporous zeolites with a carbon secondary hard template. The carbon is generated through the decomposition of methane over nickel nanoparticles. This is done as an in situ process, directly upon the silica source for the zeolite. This method is significantly cheaper than previously reported for carbon templates. This increases the feasibility of utilizing mesoporous zeolites for various applications. The mesoporous zeolite possessed a greater total pore volume, while still matching its conventional counterpart in terms of crystallinity and acidity. Samples of conventional and mesoporous zeolites were tested in a model catalytic reaction. Here, the mesoporous zeolite exhibited much higher conversion, which is contributed to the enhanced diffusion. Chapter 5 explains the fundamentals of fuel cells, as a mean to transform chemical as the main technique explained. The chapter will also cover degradation mechanisms of the catalyst employed in PEMFC, such as carbon corrosion and particle agglomeration. Strategies on how to increase resistance towards these degradation mechanisms, such as particle encapsulation, employing graphitic support, and heteroatom doping, will be described. Lastly, a possible PEMFC catalyst based on platinum dispersed on a nanoporous polymer is reported. Chapter 6 is the examination of a novel catalyst for PEMFC. The synthesis strategy aims at high durability and activity. The basis of the catalyst is the yolk-shell particles consisting of small platinum nanoparticles and a shell of nitrogen doped carbon with graphitic elements. The carbon shell will be activated with potassium hydroxide to generate some microporosity in the shell, to improve the diffusion of reactants. The catalyst is extensively characterize with respect to both the platinum nanoparticles and the carbon shell. Lastly the catalyst is employed in the electrooxidations of methanol, ethanol, and formic acid.

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry
Authors: Abildstrøm, J. O. (Intern), Kegnæs, S. (Intern), Riisager, A. (Intern)
Number of pages: 123
Publication date: 2016

Publication information
Publisher: DTU Chemistry
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
13_01910_37_Abildstroem_Thesis.pdf_2636317_1_1.pdf

Relations
Projects:
Design of porous nanostructured solid catalysts
Publication: Research › Ph.D. thesis – Annual report year: 2017

Detecting beer intake by unique metabolite patterns
Evaluation of health related effects of beer intake is hampered by the lack of accurate tools for assessing intakes (biomarkers). Therefore, we identified plasma and urine metabolites associated with recent beer intake by untargeted metabolomics and established a characteristic metabolite pattern representing raw materials and beer production as a qualitative biomarker of beer intake. In a randomized, crossover, single-blinded meal study (MSt1) 18 participants were given one at a time four different test beverages: strong, regular and non-alcoholic beers and a soft drink. Four participants were assigned to have two additional beers (MSt2). In addition to plasma and urine samples, test beverages, wort and hops extract were analyzed by UPLC-QTOF. A unique metabolite pattern reflecting beer metabolism, including metabolites derived from beer raw material (i.e. N-methyl tyramine sulfate and the sum of iso-α-acids and tricyclohumols) and production process (i.e. pyro-glutamyl proline and 2-ethyl malate) were selected to establish a compliance biomarker model for detection of beer intake based on MSt1. The model predicted the MSt2 samples collected before and up to 12 h
after beer intake correctly (AUC = 1). A biomarker model including four metabolites representing both beer raw materials and production steps provided a specific and accurate tool for measurement of beer consumption.

**General information**

State: Published
Organisations: Department of Chemistry, Organic Chemistry, University of Copenhagen, Carlsberg Research Center
Authors: Gürdeniz, G. (Ekstern), Jensen, M. G. (Ekstern), Meier, S. (Intern), Bech, L. (Ekstern), Lund, E. (Ekstern), Dragsted, L. O. (Ekstern)
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**Publication information**

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BFI (2018): BFI-level 2
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BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.34 SJR 1.705 SNIP 1.002
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.934 SNIP 1.092 CiteScore 4.45
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.945 SNIP 1.185 CiteScore 4.64
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.002 SNIP 1.256 CiteScore 5.16
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 2.027 SNIP 1.328 CiteScore 5.12
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.119 SNIP 1.267 CiteScore 5.12
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.93 SNIP 1.246
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.959 SNIP 1.206
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.993 SNIP 1.122
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.921 SNIP 1.108
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.761 SNIP 1.091
Scopus rating (2005): SJR 2.192 SNIP 1.409
Scopus rating (2004): SJR 2.298 SNIP 1.39
Scopus rating (2003): SJR 1.995 SNIP 0.944
Original language: English
Determination of Water Vapor Pressure Over Corrosive Chemicals Versus Temperature Using Raman Spectroscopy as Exemplified with 85.5% Phosphoric Acid

A method to determine the water vapor pressure over a corrosive substance was developed and tested with 85.5±0.4% phosphoric acid. The water vapor pressure was obtained at a range of temperatures from ~25°C to ~200°C using Raman spectrometry. The acid was placed in an ampoule and sealed with a reference gas (either hydrogen or methane) at a known pressure (typically ~0.5 bar). By comparing the Raman signals from the water vapor and the references, the water pressure was determined as a function of temperature. A considerable amount of data on the vapor pressure of phosphoric acid are available in the literature, to which our results could successfully be compared. A record value of the vapor pressure, 3.40 bar, was determined at 210°C. The method required a determination of the precise Raman scattering ratios between the substance, water, and the used reference gas, hydrogen or methane. In our case the scattering ratios between water and reference ν1 Q-branches were found to be 1.20±0.03 and 0.40±0.02 for H2 and CH4, respectively.
The black mamba (Dendroaspis polylepis) is one of the most feared and dangerous snakes in the world, and its bite has a very high mortality and morbidity rate. Dendrotoxins, the most abundant and some of the most toxic components present in black mamba venom, target potassium channels in neuronal tissue, leading to hyper-excitability in victims and prey. Blockage of the potassium channels can lead to respiratory paralysis and eventually death. Early administration of appropriate antivenom is the only effective snakebite therapy to date. However, current antivenoms are still being produced by the very laborious and expensive traditional animal immunization techniques, leading to severe side effects in human recipients due to their heterologous nature. In contrast, novel approaches based on synthetic or recombinant antivenoms may offer an alternative solution, saving cost, limiting side effects, and providing more effective neutralization of snake venom.

**Development of peptidic anti-dendrotoxins**

The black mamba (Dendroaspis polylepis) is one of the most feared and dangerous snakes in the world, and its bite has a very high mortality and morbidity rate. Dendrotoxins, the most abundant and some of the most toxic components present in black mamba venom, target potassium channels in neuronal tissue, leading to hyper-excitability in victims and prey. Blockage of the potassium channels can lead to respiratory paralysis and eventually death. Early administration of appropriate antivenom is the only effective snakebite therapy to date. However, current antivenoms are still being produced by the very laborious and expensive traditional animal immunization techniques, leading to severe side effects in human recipients due to their heterologous nature. In contrast, novel approaches based on synthetic or recombinant antivenoms may offer an alternative solution, saving cost, limiting side effects, and providing more effective neutralization of snake venom.

**General information**

- **State:** Published
- **Organisations:** Department of Systems Biology, Department of Chemistry, Organic Chemistry, Technical University of Denmark, University of Copenhagen
- **Authors:** Oscoz, S. (Ekstern), Laustsen, A. H. (Intern), Clausen, M. H. (Intern), Lohse, B. (Ekstern)
- **Number of pages:** 1
- **Publication date:** 2016
- **Event:** Abstract from 14th Protein.DTU Workshop, Kgs. Lyngby, Denmark.
- **Main Research Area:** Technical/natural sciences
Direct transformation of carbohydrates to the biofuel 5-ethoxymethylfurfural by solid acid catalysts

The direct conversion of glucose to 5-ethoxymethylfurfural (EMF) is a promising biomass transformation due to the products potential application as a biofuel. Here, the conversion of glucose to EMF was examined over several solid acid catalysts in ethanol between 96 and 125 °C. Among the catalysts employed, dealuminated beta zeolites [DeAl-H-beta-12.5 (700)] gave a moderate yield of EMF (37%) in a single step catalytic process. A combined catalytic system consisting of H-form zeolite and Amberlyst-15 was found to be more efficient for the transformation of glucose to EMF (46%) via an one-pot, two-step reaction protocol. Alternative biomass-based mono-, di- and polysaccharides formed also moderate to good yields of EMF with the catalytic systems, including fructose which yielded 67 % of EMF and 4% of ethyl levulinate (ELevu) along with 10 % 5-hydroxymethylfurfural (HMF) in the combined reaction protocol. A significant amount of ELevu (1-16 %), a rehydrated product of EMF and promising fuel additive, was observed in this study. Recyclability studies suggested that it was possible to reuse the DeAl-H-beta-12.5 (700) catalyst in consecutive reactions without significant changes in product yields due to its easy recovery and thermal stability during regeneration.
Dissolution Dynamic Nuclear Polarization capability study with fluid path

Signal enhancement by hyperpolarization is a way of overcoming the low sensitivity in magnetic resonance; MRI in particular. One of the most well-known methods, dissolution Dynamic Nuclear Polarization, has been used clinically in cancer patients. One way of ensuring a low bioburden of the hyperpolarized product is by use of a closed fluid path that constitutes a barrier to contamination. The fluid path can be filled with the pharmaceuticals, i.e. imaging agent and solvents, in a clean room, and then stored or immediately used at the polarizer. In this study, we present a method of filling the fluid path that allows it to be reused. The filling method has been investigated in terms of reproducibility at two extrema, high dose for patient use and low dose for rodent studies, using [1-13C]pyruvate as example. We demonstrate that the filling method allows high reproducibility of six quality control parameters with standard deviations 3–10 times smaller than the acceptance criteria intervals in clinical studies.

General information

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BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.37 SJR 0.973 SNIP 0.981
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Effect of Aluminum Substrate Surface Modification on Wettability and Freezing Delay of Water Droplet at Subzero Temperatures

In this study, we have investigated the freezing delay of a water droplet on precooled substrates of an aluminum alloy that is commonly used for heat-exchanger fins. The surfaces of the substrates were modified to obtain surfaces with different hydrophilicity/hydrophobicity and different surface chemistry but without significantly modifying the surface topography. The freezing delays and water contact angles were measured as a function of the substrate temperature and the results were compared to the predictions of the heterogeneous ice nucleation theory. Although the trends for each sample followed the trend in this theory, the differences in the extents of freezing delays were in apparent disagreement with the predictions. Concretely, a slightly hydrophilic substrate modified by (3-aminopropyl) triethoxysilane (APTES) showed longer freezing delays than both more hydrophilic and more hydrophobic substrates. We suggest that this is because this particular surface chemistry prevents ice formation at the interface of the substrate, prior to the deposition of the water droplet. On the basis of our results, we suggest that not only wettability and topography but also the concrete surface
chemistry plays a significant role in the kinetics of the ice formation process when a water droplet is placed on a precooled substrate.

**General information**

State: Published
Organisations: Department of Chemistry, Aalborg University
Authors: Rahimi, M. (Ekstern), Afshari, A. (Ekstern), Thormann, E. (Intern)
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Volume: 8
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- Web of Science (2017): Indexed yes
- BFI (2016): BFI-level 1
- Scopus rating (2016): CiteScore 7.6 SJR 2.524 SNIP 1.528
- Web of Science (2016): Indexed yes
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- Scopus rating (2015): SJR 2.299 SNIP 1.568 CiteScore 7.38
- Web of Science (2015): Indexed yes
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- Scopus rating (2014): SJR 2.126 SNIP 1.64 CiteScore 6.88
- Web of Science (2014): Indexed yes
- BFI (2013): BFI-level 1
- Scopus rating (2013): SJR 1.979 SNIP 1.543 CiteScore 6.05
- ISI indexed (2013): ISI indexed yes
- Web of Science (2013): Indexed yes
- BFI (2012): BFI-level 1
- Scopus rating (2012): SJR 2.18 SNIP 1.309 CiteScore 4.94
- ISI indexed (2012): ISI indexed yes
- Web of Science (2012): Indexed yes
- BFI (2011): BFI-level 1
- Scopus rating (2011): SJR 2.017 SNIP 1.396 CiteScore 4.41
- ISI indexed (2011): ISI indexed no
- Web of Science (2011): Indexed yes
- Scopus rating (2010): SJR 1.571 SNIP 0.931
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**Effect of tert-Butyl Functionalization on the Photoexcited Decay of a Fe(II)-N-Heterocyclic Carbene Complex**

Understanding and subsequently being able to manipulate the excited-state decay pathways of functional transition-metal complexes is of utmost importance in order to solve grand challenges in solar energy conversion and data storage. Herein, we perform quantum chemical calculations and spin-vibronic quantum dynamics simulations on the Fe-N-heterocyclic carbene complex, [Fe(btbip)]Z2+ (btbip = 2,6-bis(3-tert-butyl-imidazole-1-ylidene)pyridine). The results
demonstrate that a relatively minor structural change compared to its parent complex, \([\text{Fe(bmip}_2]^{2+} (\text{bmip} = 2,6\text{-bis(3-methyl-imidazole-1-ylidene)pyridine}), completely alters the excited-state relaxation. Ultrafast deactivation of the initially excited metal-to-ligand charge transfer (1,3MLCT) states occurs within 350 fs. In contrast to the widely adopted mechanism of Fe(II) photophysics, these states decay into close-lying singlet metal-centered (1MC) states. This occurs because the tert-butyl functionalization stabilizes the 1MC states, enabling the 1,3MLCT \rightarrow 1MC population transfer to occur close to the Franck-Condon geometry, making the conversion very efficient. Subsequently, a spin cascade occurs within the MC manifold, leading to the population of triplet and quintet MC states. These results will inspire highly involved ultrafast experiments performed at X-ray free electron lasers and shall pave the way for the design of novel high-efficiency transition-metal-based functional molecules.

**General information**

State: Published
Organisations: Department of Chemistry, Department of Chemistry, Newcastle University
Authors: Pápai, M. I. (Intern), Penfold, T. J. (Ekstern), Møller, K. B. (Intern)
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Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.48 SJR 1.948 SNIP 1.181
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.917 SNIP 1.268 CiteScore 4.68
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.027 SNIP 1.448 CiteScore 5.08
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 2.134 SNIP 1.439 CiteScore 5.14
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.514 SNIP 1.46 CiteScore 4.98
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.32 SNIP 1.457 CiteScore 4.92
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 2.438 SNIP 1.356
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 2.128 SNIP 1.417
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.856 SNIP 1.033
Effects of strong cathodic polarization of the Ni-YSZ interface

Long-term strong cathodic polarization experiments of down to -2.4 V vs. E°(O₂) of the Ni-YSZ interface were performed at 900°C in 97% H₂/3% H₂O on model electrodes. The Ni-YSZ interface underwent extensive changes and a large affected volume with a complex microstructure and phase distribution resulted. Impedance spectroscopy shows initial decrease but later increase in the series resistance and polarization resistance during the 140-160 h of polarization, and significant inductive behavior. An intermetallic Ni-Zr phase that formed during polarization was preserved when the polarization was kept during cooling, and was identified post-mortem by transmission electron microscopy as Ni₇Zr₂. ZrO₂ nanoparticles were formed on the Ni-gas surface next to the Ni-YSZ-gas triple phase boundary. Explanations of the observed features are offered based on electron microscopy and impedance spectroscopy.
Efficient Aerobic Oxidation of 5-Hydroxymethylfurfural in Aqueous Media with Au-Pd Supported on Zinc Hydroxycarbonate

Bimetallic catalysts with Au–Pd supported on zinc hydroxycarbonate (ZOC) were synthesized by a simple deposition–precipitation method and analyzed by transmission electron microscopy to have a narrow-size distribution of predominantly 1–2 nm. The prepared Au–Pd/ZOC catalysts exhibited excellent activity towards 5-hydroxymethylfurfural (HMF) oxidation in water in the presence of the base NaHCO3 at benign conditions of 80 °C and 3 bar O2, resulting in quantitative yield of 2,5-furandicarboxylic acid (FDCA). The addition of base not only enhanced the yield of FDCA but also stabilized the support ZOC by preventing ZOC from the reaction with formed carboxylic acid intermediates/products, thus allowing Au–Pd/ZOC to be recycled for at least six times without significant loss of activity. The basicity of ZOC could play an important role in obtaining the improved yield of FDCA as compared to other supports.
Efficient hydrogen peroxide decomposition to oxygen and water catalysed by a ruthenium pincer complex

Hydrogen peroxide decomposition is a major issue in medicine, energy, and environmental sciences. For example, findings could lead to the development of efficient H$_2$O$_2$ removal systems to clean wastewaters. Here I tested several homogeneous catalysts for H$_2$O$_2$ decomposition. I found that a dihydride version of a ruthenium complex coordinated by a phosphorous–nitrogen–phosphorus pincer ligand with isopropyl substituents on the phosphorus (PNPiPr) was superior to the hydride chloride congener. This is in line with previous activity studies with PNPiPr ruthenium catalysts. Moreover, no additives are necessary, further enhancing the potential scope of this system. By the use of the homogeneous catalyst Ru(H)$_2$(PNPiPr)CO, it is possible to obtain turnover frequencies reaching 180,000 h$^{-1}$ and turnover numbers more than 14,000 in a neutral hydrogen peroxide aqueous solution at 25 °C. Overall, findings reveal an efficient and stable system for hydrogen peroxide decomposition to oxygen and water under mild conditions.
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)
Pages: 3942-3945
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Electronic versions:
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Electrocatalytic Applications of Graphene–Metal Oxide Nanohybrid Materials

Development of state-of-the-art electrocatalysts using commercially available precursors with low cost is an essential step in the advancement of next-generation electrochemical energy storage/conversion systems. In this regard, noble metal-free and graphene-supported nanocomposites are of particular interest. Graphene-based nanocomposite is an excellent candidate as energy-device and sensor-related electrode materials, largely due to their high electrical conductivity, large specific surface area, high-speed electron/heat mobility, and reasonably good mechanical strength. Among many types of graphene-based composite materials, graphene–metal oxide nanohybrids hold great promise to ward engineering efficient electrocatalysts and have attracted increasing interest in both scientific communities and industrial partners around the world. The goal of this chapter is primarily set on an overview of cutting-edge developments in graphene–metal oxide nanohybrid materials, with the recently reported results from worldwide research groups. This chapter is presented first with an introduction, followed by synthetic methods and structural characterization of nanocomposites, an emphasis on their applications in energy and sensor-related fields, and finally completed with brief conclusions and outlook.

General information
State: Published
Organisations: Department of Chemistry, NanoChemistry, Organic Chemistry
Authors: Halder, A. (Intern), Zhang, M. (Intern), Chi, Q. (Intern)
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Title of host publication: Advanced Catalytic Materials : Photocatalysis and Other Current Trends
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Chapter: 14
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Electrochemically active functionalization of graphene for development of prototype biosensing devices

Development of low-cost, robust and ultra-sensing material platforms for clinically important analytes is one of the key steps for new-generation biosensors. As a promising 2D material, graphene has emerged to fulfill such purposes. Graphene based materials have shown the potential to be an ideal support for chemosensors and biosensors. Functionalization of graphene can further transform this 2D material into various versatile platforms for different applications. In this presentation, we will address some of our recent investigations: (1) electrochemically active functionalization of graphene nanosheets, (2) loading of different enzymes on functionalized graphene matrix, and (3) electrochemical performances of the functionalized nano-organic hybrid materials based prototype sensors. These latest advancements could be crucial for the design and fabrication of low-cost, flexible and disposable biosensors.

Electrochemistry of Hemin on Single-Crystal Au(111)-electrode Surfaces

Iron porphyrin, hemin (Fig. 1A), is the active core in cytochromes, haemoglobin and myoglobin, and enzymes such as the peroxidases. These metalloproteins are engaged in respiratory electron transfer, oxygen transport and storage, and enzyme catalysis in the biosynthesis of a range of metabolites. Hemin itself also acts as catalyst in electrochemical reduction of dioxygen and other small inert molecules such as nitrogen monoxide, and in electrochemiluminescent detection of dioxygen, peroxide, DNA, and proteins. n-n interactions of hemin with carbon materials have been broadly studied. Hemin on noble metalsurfaces has been prime targets in high-resolution STM but much less used in applied contexts such as biosensors and drug delivery. How hemin molecules interact with noble metal surfaces offers, however, other challenges in nanoscale and single-molecule science. We have studied hemin adsorption on well-defined single-crystal Au(111)-electrode surfaces using electrochemistry combined with scanning tunnelling microscopy under electrochemical control. Hemin gives two voltammetric peaks assigned to adsorbed monomers and dimmers (Fig. 1B). In situ STM shows that hemin self-assembles in ordered monolayers through non-covalent adsorption, as the reconstruction of the Au-(111) surface underneath the hemin layer is clearly visible (Fig. 1C).

Electron Transfer and Solvent-Mediated Electronic Localization in Molecular Photocatalysis

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

**General information**

State: Published
Organisations: Department of Chemistry, Department of Physics, Neutrons and X-rays for Materials Physics, University of Hamburg
Authors: Dohn, A. O. (Intern), Kjaer, K. S. (Intern), Harlang, T. B. (Ekstern), Canton, S. E. (Ekstern), Nielsen, M. M. (Intern), Møller, K. B. (Intern)
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.64 SJR 1.774 SNIP 1.198
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.805 SNIP 1.239 CiteScore 4.7
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.869 SNIP 1.314 CiteScore 4.69
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.819 SNIP 1.379 CiteScore 4.9
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 2.08 SNIP 1.35 CiteScore 4.72
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.952 SNIP 1.373 CiteScore 4.64
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.98 SNIP 1.323
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.982 SNIP 1.47
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 2.025 SNIP 1.412
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 2.136 SNIP 1.544
Elucidating the Ultrafast Dynamics of Photoinduced Charge Separation in Metalloporphyrin-Fullerene Dyads Across the Electromagnetic Spectrum

Metalloporphyrins are prominent building blocks in the synthetic toolbox of advanced photodriven molecular devices. When the central ion is paramagnetic, the relaxation pathways within the manifold of excited states are highly intricate so that unravelling the intramolecular energy and electron transfer processes is usually a very complex task. This fact is critically hampering the development of applications based on the enhanced coupling offered by the electronic exchange interaction. In this work, the dynamics of charge separation in a copper porphyrin-fullerene are studied with several complementary spectroscopic tools across the electromagnetic spectrum (from near-infrared to X-ray wavelengths), each of them providing specific diagnostics. Correlating the various rates clearly demonstrates that the lifetime of the photoinduced charge-separated state exceeds by about 10-fold that of the isolated photoexcited CuII porphyrin. As revealed by the spectral modifications in the XANES region, this stabilization is accompanied by a transient change in covalency around the CuII center, which is induced by an enhanced interaction with the C60 moiety. This experimental finding is further confirmed by state-of-the-art calculations using DFT and TD-DFT including dispersion effects that explain the electrostatic and structural origins of this interaction, as the CuII cation becomes ruffled and approaches closer to the fullerene in the charge-separated state. From a methodological point of view, these results exemplify the potential of multielectron excitation features in transient X-ray spectra as future diagnostics of subfemtosecond electronic dynamics. From a practical point of view, this work is paving the way for elucidating out-of-equilibrium electron transfer events coupled to magnetic interaction processes on their intrinsic time-scales.

General information
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Organisations: Department of Chemistry, Tianjin Polytechnic University, Friedrich-Alexander Universität, Argonne National Laboratory, Uppsala University, Deutsches Elektronen-Synchrotron
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Enhanced microbial electrosynthesis with three-dimensional graphene functionalized cathodes fabricated via solvothermal synthesis

The biological reduction of CO$_2$ into multicarbon chemicals can be driven by electrons derived from the cathode of a bioelectrochemical reactor via microbial electrosynthesis (MES). To increase MES productivity, conditions for optimal electron transfer between the cathode and the microbial catalyst must be implemented. Here, we report the development
of a 3D-graphene functionalized carbon felt composite cathode enabling faster electron transfer to the microbial catalyst Sporomusa ovata in a MES reactor. Modification with 3D-graphene network increased the electrosynthesis rate of acetate from CO₂ by 6.8 fold. It also significantly improved biofilm density and current consumption. A 2-fold increase in specific surface area of the 3D-graphene/carbon felt composite cathode explained in part the formation of more substantial biofilms compared to untreated control. Furthermore, in cyclic voltammetry analysis, 3D-graphene/carbon felt composite cathode exhibited higher current response. The results indicate that the development of a 3D-network cathode is an effective approach to improve microbe-electrode interactions leading to productive MES systems.

General information
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Organisations: Novo Nordisk Foundation Center for Biosustainability, Research Groups, Bioelectrochemical Systems, Department of Chemistry, NanoChemistry, Organic Chemistry
Authors: Aryal, N. (Intern), Halder, A. (Intern), Tremblay, P. (Intern), Chi, Q. (Intern), Zhang, T. (Intern)
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BFI (2018): BFI-level 2
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Scopus rating (2016): CiteScore 4.74 SJR 1.357 SNIP 1.167
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.349 SNIP 1.344 CiteScore 4.86
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.391 SNIP 1.482 CiteScore 4.59
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.435 SNIP 1.607 CiteScore 4.44
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.651 SNIP 1.592 CiteScore 3.99
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.621 SNIP 1.803 CiteScore 4.15
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.691 SNIP 1.725
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.536 SNIP 1.625
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.533 SNIP 1.47
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.563 SNIP 1.595
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.534 SNIP 1.736
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.481 SNIP 1.533
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.365 SNIP 1.581
Scopus rating (2003): SJR 1.628 SNIP 1.526
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 1.644 SNIP 1.459
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 1.319 SNIP 1.408
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Scopus rating (2000): SJR 1.009 SNIP 1.168
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Bioelectrochemical system, Carbon dioxide fixation, Cathode electrode, Graphene, Microbial electrosynthesis

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En ny historie om guld og svovl - guld-svovlbindningen i thiolers adsorption på guldnanopartikler og plane guldoverflader

General information
State: Published
Organisations: Department of Chemistry, NanoChemistry, Organic Chemistry, University of Technology, Sydney, University of Sydney
Authors: Chi, Q. (Intern), Ford, M. J. (Ekstern), Halder, A. (Intern), Hush, N. S. (Ekstern), Reimers, J. R. (Ekstern), Ulstrup, J. (Intern), Zhang, J. (Intern)
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Enzymatic Modifications Based on the Surroundings of Cofactor

General information
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Organisations: Department of Chemistry, NanoChemistry, Organic Chemistry
Authors: Zhang, L. (Intern), Ulstrup, J. (Intern), Zhang, J. (Intern)
Number of pages: 1
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Main Research Area: Technical/natural sciences
Evidence for a hopping mechanism in metal|single molecule|metal junctions involving conjugated metal–terpyridyl complexes; potential-dependent conductances of complexes [M(pyterpy)2]2+(M = Co and Fe; pyterpy = 4′-(pyridin-4-yl)-2,2′:6′,2′′-terpyridine) in ionic liquid

Extensive studies of various families of conjugated molecules in metal|molecule|metal junctions suggest that the mechanism of conductance is usually tunnelling for molecular lengths < ca. 4 nm, and that for longer molecules, coherence is lost as a hopping element becomes more significant. In this work we present evidence that, for a family of conjugated, redox-active metal complexes, hopping may be a significant factor for even the shortest molecule studied (ca. 1 nm between contact atoms). The length dependence of conductance for two series of such complexes which differ essentially in the number of conjugated 1,4-C6H4- rings in the structures has been studied, and it is found that the junction conductances vary linearly with molecular length, consistent with a hopping mechanism, whereas there is significant deviation from linearity in plots of log(conductance) vs. length that would be characteristic of tunnelling, and the slopes of the log(conductance)–length plots are much smaller than expected for an oligophenyl system. Moreover, the conductances of molecular junctions involving the redox–active molecules, [M(pyterpy)2]2+/3+ (M = Co, Fe) have been studied as a function of electrochemical potential in ionic liquid electrolyte, and the conductance–overpotential relationship is found to fit well with the Kuznetsov–Ulstrup relationship, which is essentially a hopping description.
Extracellular polymeric substances play roles in extracellular electron transfer of Shewanella oneidensis MR-1

It is well known that microorganism is surrounded by extracellular polymeric substances (EPS) which include polysaccharides, proteins, glycoproteins, nucleic acids, phospholipids, and humic acids. However, previous studies on microbial extracellular electron transfer (EET) are conducted on cells without extracting EPS or cells collected from log stage or early-steady stage cultures with little EPS. Therefore, microbial cells are believed in contact directly with each other or electrode. Such attempt apparently ignored the role of EPS in microbial EET, even though many components of EPS, such as DNA, humic acids and some proteins, are electrochemically active or semiconductive. Herein, we report experimental evidences of EPS role on EET for Shewanella oneidensis MR-1.

Atomic force microscopy clearly showed that the cell surface was cleaned and few EPS could be observed on MR-1 after the extraction (Figure 1.a and 1.b). Comparing to cells in control group, MR-1 treated at 38 °C for EPS extraction showed different electrochemical characterizations as revealed by differential pulse voltammetry (Figure 1.c). EPS extracted from MR-1 also was proved to be electrochemically active. The present study indicated that EPS play important roles in EET of MR-1.

General information
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Organisations: Department of Chemistry, NanoChemistry, Metalloprotein Chemistry and Engineering, Organic Chemistry, Chinese Academy of Sciences
Authors: Xiao, Y. (Intern), Zhang, E. (Ekstern), Christensen, H. E. M. (Intern), Zhang, J. (Intern), Zhao, F. (Ekstern)
Number of pages: 1
Event: Abstract from 3rd European Meeting of the International Society for Microbial Electrochemistry and Technology (EU-ISMET 2016), Rome, Italy.
Main Research Area: Technical/natural sciences
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Abstract_Yong_Xiao.pdf
Source: PublicationPreSubmission
Source-ID: 128888450
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2017
Femtosecond X-Ray Scattering Study of Ultrafast Photoinduced Structural Dynamics in Solvated [Co(terpy)$_2$]$_2^{2+}$

We study the structural dynamics of photoexcited [Co(terpy)$_2$]$_2^{2+}$ in an aqueous solution with ultrafast x-ray diffuse scattering experiments conducted at the Linac Coherent Light Source. Through direct comparisons with density functional theory calculations, our analysis shows that the photoexcitation event leads to elongation of the Co-N bonds, followed by coherent Co-N bond length oscillations arising from the impulsive excitation of a vibrational mode dominated by the symmetrical stretch of all six Co-N bonds. This mode has a period of 0.33 ps and decays on a subpicosecond time scale. We find that the equilibrium bond-elongated structure of the high spin state is established on a single-picosecond time scale and that this state has a lifetime of ~7 ps.

General information
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Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Theoretical Atomic-scale Physics, Department of Chemistry, Lund University
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BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
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Scopus rating (2016): CiteScore 6.33 SJR 3.56 SNIP 2.133
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 3.823 SNIP 2.205 CiteScore 5.76
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 5.027 SNIP 2.646 CiteScore 6.62
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 5.674 SNIP 2.796 CiteScore 7.46
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 6.243 SNIP 2.845 CiteScore 7.19
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 6.252 SNIP 2.886 CiteScore 7.02
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 6.418 SNIP 2.764
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 6.342 SNIP 2.94
Web of Science (2009): Indexed yes
Flavins mediate extracellular electron transfer in Gram-positive Bacillus megaterium strain LLD-1
Electrochemically active microorganisms are microbes which can transfer electrons from cell to extracellular electron acceptors such as minerals, contaminants, electrodes, etc., and these processes are defined as extracellular electron transfer. In this study, we isolated and identified a new electrochemically active strain of Bacillus megatherium strain LLD-1, and its extracellular electron transfer mechanism was demonstrated by cyclic voltammetry (CV), differential pulse voltammetry (DPV), HPLC, and chronamperometric.

The CV and DPV showed that a redox peaks ascribing to membrane proteins was found in the strain LLD-1; another redox peaks observed in cell and supernatant were ascribed to flavins. 74% increment of voltage generation in LLD-1 inoculated microbial fuel cell (MFC) can be made by adding extra 0.1 μM flavins mixture solution.

Formation and reactivity of nitrates on Cu(II) sites in copper substituted CHA zeolite
Electrochemically active microorganisms are microbes which can transfer electrons from cell to extracellular electron acceptors such as minerals, contaminants, electrodes, etc., and these processes are defined as extracellular electron transfer. In this study, we isolated and identified a new electrochemically active strain of Bacillus megatheterium strain LLD-1, and its extracellular electron transfer mechanism was demonstrated by cyclic voltammetry (CV), differential pulse voltammetry (DPV), HPLC, and chronamperometric.

The CV and DPV showed that a redox peaks ascribing to membrane proteins was found in the strain LLD-1; another redox peaks observed in cell and supernatant were ascribed to flavins. 74% increment of voltage generation in LLD-1 inoculated microbial fuel cell (MFC) can be made by adding extra 0.1 μM flavins mixture solution.
Free-standing and flexible graphene papers as disposable non-enzymatic electrochemical sensors

We have explored AuNPs (13 nm) both as a catalyst and as a core for synthesizing water-dispersible and highly stable core-shell structural gold@Prussian blue (Au@PB) nanoparticles (NPs). Systematic characterization by transmission electron microscopy (TEM) and X-ray photoelectron spectroscopy (XPS) disclosed AuNPs coated uniformly by a 5 nm thick PB layer. Au@PB NPs were attached to single-layer graphene oxide (GO) to form Au@PB decorated GO sheets. The resulting hybrid material was filtered layer-by-layer into flexible and freestanding GO paper, which was further converted into conductive reduced GO (RGO)/Au@PB paper via hydrazine vapour reduction. High-resolution TEM images suggested that RGO papers are multiply sandwich-like structures functionalized with core-shell NPs. Resulting sandwich functionalized graphene papers have high conductivity, sufficient flexibility, and robust mechanical strength, which can be cut into free-standing electrodes. Such electrodes, used as non-enzymatic electrochemical sensors, were tested systematically for electrocatalytic sensing of hydrogen peroxide. The high performance was indicated by some of the key parameters, for example the linear H₂O₂ concentration response range (1-30 μM), the detection limit (100 nM), and the high amperometric sensitivity (5 A cm⁻² M⁻¹). With the advantages of low cost and scalable production capacity, such graphene supported functional papers are of particular interest in the use as flexible disposable sensors.

General information

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Organisations: Department of Chemistry, NanoChemistry, Organic Chemistry
Authors: Zhang, M. (Intern), Halder, A. (Intern), Hou, C. (Intern), Ulstrup, J. (Intern), Chi, Q. (Intern)
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Scopus rating (2016): CiteScore 3.45 SJR 0.751 SNIP 0.996
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.813 SNIP 1.383 CiteScore 3.76
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.115 SNIP 1.402 CiteScore 4.25
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.947 SNIP 1.389 CiteScore 3.81
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.255 SNIP 1.386 CiteScore 4.06
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Graphene paper, Electrochemistry, Disposable sensors, Flexible 2D materials, Electroactive nanoparticles, Core/shell nanoparticles

From single cells to single molecules: general discussion

State: Published
Organisations: Department of Chemistry, NanoChemistry

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Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
General Approach to Characterize Reservoir Fluids Using a Large PVT Database

Global increase in oil demand has resulted in the need for exploring remote and harsh locations where a considerable portion of them are at extreme reservoir temperatures and pressures. Accurate calculation of properties of gas and oil at high pressures and high temperatures (HPHT) is a more prominent issue. Non-cubic Equation of State (EoS) models are an attractive option due to their better description of density and compressibility over a wide temperature and pressure range. Application of these models to reservoir fluids requires development of the corresponding fluid characterization methods. We proposed a general approach to develop correlations for model parameters and applied it to the characterization for the PC-SAFT EoS. The approach consists in first developing the correlations based on the DIPPR database, and then adjusting the correlations based on a large PVT database. The adjustment was made to minimize the deviation in key PVT properties like saturation pressures, densities at reservoir temperature and Stock Tank Oil (STO) densities, while keeping the n-alkane limit of the correlations unchanged. As an improvement of a previously suggested characterization method, the approach gives better PVT calculation results for the tested systems. Comparison was also made between PC-SAFT with the proposed characterization method and other EoS models. The proposed approach can
be applied to other EoS models for improving their fluid characterization. Besides, the challenges with PNA based characterization methods are discussed.

**Glucuronic Acid Derivatives in Enzymatic Biomass Degradation: Synthesis and Evaluation of Enzymatic Activity**

An essential tool for biotechnology companies in enzyme development for biomass delignification is the access to well-defined model substrates. A deeper understanding of the enzymes substrate specificity can be used to address and optimize enzyme mixtures towards natural, complex substrates. Hence, the chemically synthesized substrates often outcompete those isolated from natural sources in terms of reproducibility, homogeneity and purity.

The first part of this work was the synthesis of two glucuronoxylan fragments designed as model substrates for xylanases. The synthesis involved the use of thioxyloside building blocks in an iterative, linear glycosylation strategy. Two sidechain glucuronate building blocks were synthesized via a divergent strategy from the same thioethylglucose derivative.

In the second part of the project three alkylaromatic and aromatic esters have been prepared as mimics of lignin-carbohydrate complexes found in lignocellulosic biomass, as model substrates for glucuronoyl esterases (GEs). These esters have been used to characterize a novel GE from Cerrena unicolor (CuGE), produced by Novozymes, to obtain insights into the substrate specificity of the enzymes. HPLC analysis of the enzymatic reactions led to the determination of kinetic parameters that gave information about both bonding affinity and catalytic efficiency.

**Glycosylation with Disarmed Glycosyl Bromides Promoted by Iodonium Ions**

Iodonium ions have been developed for activating glycosyl bromides in the coupling to glycosyl acceptors. The iodonium ions are generated from N-iodosuccinimide and a protic acid such as camphorsulfonic acid or triflic acid, where the latter gives the most reactive promoter system. The couplings occur with the release of iodine monobromide, and the best results are obtained with benzoylated glycosyl donors and acceptors. In this way, disarmed glycosyl bromides can serve as glycosyl donors without the use of heavy-metal salts.
Gold surfaces and nanoparticles are protected by Au(0)-thiyl species and are destroyed when Au(I)-thiolates form. The synthetic chemistry and spectroscopy of sulfur-protected gold surfaces and nanoparticles is analyzed, indicating that the electronic structure of the interface is Au(0)-thiyl, with Au(I)-thiolates identified as high-energy excited surface states. Density-functional theory indicates that it is the noble character of gold and nanoparticle surfaces that destabilizes Au(I)-thiolates. Bonding results from large van der Waals forces, influenced by covalent bonding induced through s-d hybridization and charge polarization effects that perturbatively mix in some Au(I)-thiolate character. A simple method for quantifying these contributions is presented, revealing that a driving force for nanoparticle growth is nobleization, minimizing Au(I)-thiolate involvement. Predictions that Brust-Schiffrin reactions involve thiolate anion intermediates are verified spectroscopically, establishing a key feature needed to understand nanoparticle growth. Mixing of preprepared Au(I) and thiolate reactants always produces Au(I)-thiolate thin films or compounds rather than monolayers. Smooth links to O, Se, Te, C, and N linker chemistry are established.
Main Research Area: Technical/natural sciences

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Web of Science (2018): Indexed yes
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Scopus rating (2016): CiteScore 8.56 SJR 6.321 SNIP 2.629
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 6.767 SNIP 2.682 CiteScore 8.84
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 6.853 SNIP 2.725 CiteScore 8.86
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 6.989 SNIP 2.73 CiteScore 9.5
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 6.792 SNIP 2.682 CiteScore 9.49
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 6.771 SNIP 2.636 CiteScore 9.31
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 6.769 SNIP 2.529
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 6.913 SNIP 2.544
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 6.899 SNIP 2.445
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 6.766 SNIP 2.441
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 6.734 SNIP 2.434
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 6.784 SNIP 2.551
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 7.026 SNIP 2.622
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 7.018 SNIP 2.501
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 7.183 SNIP 2.471
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 7.192 SNIP 2.463
Graphene-Metal Oxide Hybrid Nanostructured Materials for Electrocatalytic Sensing and Sustainable Energy Storage

Graphene based materials have attracted tremendous attention, attributed to their unique physicochemical properties and versatile applications. In general, these materials are very promising candidates for the development of next-generation electrochemical systems for energy and environmental technology and sensor applications. In particular, graphene-metal oxide nanohybrid materials have been introduced as a new basis for preparation of low cost and highly efficient electrocatalysts for energy storage and conversion as well as for electrochemical sensing applications. By combining graphene with specific metal oxide nanostructures, resulting nanohybrid materials can play a significant role in the cutting-edge development of state-of-the-art electrocatalysts using commercially available and low-cost precursors. Herein, we review the mostly recent advances in the development of noble metal free graphene supported electrocatalysts. This review includes an introduction to graphene-metal oxide based nanohybrid materials, different synthetic strategies for the preparation of graphene/metal oxide nanocomposites and their structural characterization, and an overview of various electrochemical applications. The current challenges and possible future directions are briefly discussed, prior to conclusions.

Graphene paper based bioelectrodes for enzymatic biofuel cells

We aim at developing bioelectrodes for enzymatic biofuel cells, where sustainable and renewable enzymes are used for catalyzing the oxidation and reduction of fuel molecules. Here glucose is chosen as fuel molecule and glucose oxidase (GOx) is target enzyme which catalyzes the oxidation of glucose. Due to its large surface area, good electronic conductivity and biocompatibility, 3-dimensional graphene paper is used as supporting electrode material to accommodate GOx. In addition, graphene paper is flexible with good mechanic strength and an ideal fit for bioelectrodes. The graphene paper based GOx electrode is made through formation of graphene oxide, graphene paper and immobilization of GOx on the graphene paper. The prepared bioelectrodes have been measured by electrochemistry and scanning electron microscopy.
microscopy (SEM). Cyclic voltammetry show clearly electrocatalytic signals for oxidation of glucose. This indicates that the enzyme has been successfully immobilized and is actively consuming glucose while transferring electrons to the graphene paper-GOx bioanode. Stability and efficiency of the bioelectrodes are under investigation.

**Graphene Paper Based Nanomaterials for Electrochemical Sensing and Energy Conversion**

Graphene has emerged as a highly interesting material since it was experimentally isolated for the first time in 2004. This single-atom-thick nanosheet consisting of carbon atoms arrayed in a honeycomb pattern, displays outstanding physiochemical properties, including as an excellent conductor of heat and electricity, large specific surface area, and high mechanical strength. Therefore, graphene-based materials are expected to have great potential for use in the fields of sensors, catalysis, and as electrode materials for energy storage and conversion. In order to link practical applications of graphene-based materials to real-world, graphene nanosheets must be assembled into macroscopic architecture with desired structures and functionality. To this end, graphene oxide (GO) is a very useful building block because it contains a significant number of oxygen-containing groups on the planar surface and at the edges. These functional groups offer various possibilities for functionalization and assembly of GO nanosheets into 2D graphene films, papers or membranes with controlled macroscopic shapes. Resulting 2D graphene films/papers/membranes can be used as ideal scaffolds for the further incorporation of functional materials with specific desired functionality. The advantages of light-weight, high flexibility, large specific surface area, tough mechanical strength, and high electrical conductivity ensure graphene-based architectures holding a wide range of applications particularly associated with sensor and energy technologies. This PhD project is devoted to the synthesis, characterization, and applications of graphene paper-based nanomaterials for electrochemical sensors and energy conversion. The thesis is divided into three parts with 8 chapters in total. In Chapter 1, we provide an overview of the functional macroscopic graphene materials covering three key aspects: a) how to prepare 2D graphene films/papers, b) how to functionalize them with either polymers or other nanoscale objects, and c) what are their promising applications in the fields of molecular sieving purification, biomimetics, as flexible substrates, sensors and electrochemical energy devices. This is followed by an outline of the main experimental techniques and means used in the project (Chapter 2). In Chapters 3-5, the focus is on graphene-Prussian Blue (PB) composite materials. GO or graphene paper was functionalized by PB nanostructures including nanoparticles and interlocked PB cubes. A wide range of advanced techniques such as XRD, XPS, TEM, and SEM were employed to characterize the nanocomposites. The nanocomposites were tested for the detection of hydrogen peroxide (H2O2). Graphene paper was finally explored as a sacrificial template for the synthesis of 2D ultra-fined nanostructured porous metal oxide (MO), as described in Chapters 6-8. In Chapter 6, we demonstrated that crystalline MO can be prepared by using GO papers as sacrificial templates, and furthermore layer-by-layer, nonporous and ultrathin 2D CuO nanosheets were assembled into flexible and ultralight papers as a photocathode used for photoelectrochemical catalysis of hydrogen evolution reaction. In Chapters 7 and 8, CuO-ZnO hybrid nanosheets and NiO nanosheets were synthesized, characterized and used in the fabrication of non-enzymatic electrochemical sensors for high-performance detection of glucose and urea, respectively.
Halide-mediated regioselective 6-O-glycosylation of unprotected hexopyranosides with perbenzylated glycosyl bromide donors

The regio- and stereoselective glycosylation at the 6-position in 2,3,4,6-protected hexopyranosides has been investigated with dibutyltin oxide as the directing agent. Perbenzylated hexopyranosyl bromides were employed as the donors and the glycosylations were promoted by tetrabutylammonium bromide. The couplings were completely selective for both glucose and galactose donors and acceptors as long as the stannylene acetal of the acceptor was soluble in dichloromethane. This gave rise to a number of 1,2-cis-linked disaccharides in reasonable yields. Mannose donors and acceptors, on the other hand, did not react in the glycosylation under these conditions.

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry
Authors: Niedbal, D. A. (Intern), Madsen, R. (Intern)
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Pages: 415-419
Publication date: 2016
Main Research Area: Technical/natural sciences
Handling and Sensing of Single Enzyme Molecules: From Fluorescence Detection towards Nanoscale Electrical Measurements

Classical methods to study single enzyme molecules have provided valuable information about the distribution of conformational heterogeneities, reaction mechanisms, and transients in enzymatic reactions when individual molecules instead of an averaging ensemble are studied. Here, we highlight major advances in all-electrical single enzyme studies with a focus on recent micro- and nanofluidic tools, which offer new ways of handling and studying small numbers of molecules or even single enzyme molecules. We particularly emphasize nanofluidic devices, which enable the integration of electrochemical transduction and detection.

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Organisations: Department of Chemistry, NanoChemistry, University of Groningen, University of Twente, Delft University of Technology
Authors: Mathwig, K. (Ekstern), Chi, Q. (Intern), Lemay, S. G. (Ekstern), Rassaei, L. (Ekstern)
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Publication date: 2016
Main Research Area: Technical/natural sciences

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Journal: ChemphysChem
Heme: From quantum spin crossover to oxygen manager of life

The review discusses how the electronic structure of heme explains its central importance to oxygen-based life on Earth. Emphasis is on the chemical bonding of heme, its spin crossover, reversible \( \text{O}_2 \) binding, and \( \text{O}-\text{O} \) bond activation, put in relation to its physiological functions. The review discusses the spectroscopic and computational data that have helped to elucidate the nature of this remarkable molecular system, how it works, and how it is tuned by a range of molecular strategies. This tuning enables heme to carry out the two essential functions required for oxygen management of life, i.e. reversible oxygen binding for transport and storage, and oxygen activation for use in catalytic processes.
High Catalysis Activity of Cu2O Microcrystals to the Electrochemiluminescence of Luminol and H2O2

Cuprous oxide (Cu2O) is a classical p-type semiconductor with a direct band gap of 2.17 eV, which is widely used for solar energy conversion, CO oxidation, and photo catalytic water splitting for the low cost and environmental friendliness. For the energy band positions are favorable to the hydrogen evolution and oxygen evolution potentials, Cu2O materials also catalyze the reduction of hydrogen peroxide (H2O2), which is critical molecule in the body's metabolism processes or the industrial catalysis reactions. To improve detection sensitivity of H2O2, people have composed Cu2O materials with Ag nanoparticles or graphene nanosheets, which are sophisticated and costly. Herein, we use the electrochemiluminescence (ECL) method to improve the sensitivity of the reaction catalyzed by Cu2O microcrystals. As shown by Figure 1A, the ECL reaction of H2O2 and luminol catalyzed by Cu2O octahedra (Figure 1B) is strong at the potential of –0.2 V (vs. Ag/AgCl). And the corresponding current of the reaction is not obvious (Figure 1A, inset). We also check the effect of copper ions (Cu2+) to the ECL reaction, and there is much lower catalytic activity to the ECL reaction by Cu2+ ions. It indicates that Cu2O semiconductor microcrystal possess the good catalytic performance to this ECL reaction, which is important to develop the high-efficient and low-cost biosensors.
High temperature conductance mapping for correlation of electrical properties with micron-sized chemical and microstructural features

High temperature AC conductance mapping is a scanning probe technique for resolving local electrical properties in microscopic areas. It is especially suited for detecting poorly conducting phases and for ionically conducting materials such as those used in solid oxide electrochemical cells. Secondary silicate phases formed at the edge of lanthanum strontium manganite microelectrodes are used as an example for correlation of chemical, microstructural and electrical properties with a spatial resolution of 1–2 µm to demonstrate the technique. The measurements are performed in situ in a controlled atmosphere high temperature scanning probe microscope at 650°C in air.

General information
High temperature polymer electrolyte membrane fuel cells: Approaches, status, and perspectives

This book is a comprehensive review of high-temperature polymer electrolyte membrane fuel cells (PEMFCs). PEMFCs are the preferred fuel cells for a variety of applications such as automobiles, cogeneration of heat and power units, emergency power and portable electronics. The first 5 chapters of the book describe rationalization and illustration of approaches to high temperature PEM systems. Chapters 6 - 13 are devoted to fabrication, optimization and characterization of phosphoric acid-doped polybenzimidazole membranes, the very first electrolyte system that has demonstrated the concept of and motivated extensive research activity in the field. The last 11 chapters summarize the state-of-the-art of technological development of high temperature-PEMFCs based on acid doped PBI membranes including catalysts, electrodes, MEAs, bipolar plates, modelling, stacking, diagnostics and applications.

Hofmeister effect on thermo-responsive poly(propylene oxide) in H2O and D2O

The Hofmeister effect of NaSCN, NaCl and NaF on poly(propylene oxide) solutions in H2O and D2O is studied. The effect of the solvent substitution is shown to vary for different salts and we suggest that this is due to a change in the polymer accessible surface area and ion hydration.
Although a vast amount of research has been dedicated to investigate the Hofmeister effect on the stability of polymer solutions, a clear understanding of the role of polymer properties in this phenomenon is still missing. Here, the Hofmeister effect of NaCl (destabilizing) and NaSCN (stabilizing) salts on aqueous solutions of poly(propylene oxide) (PPO) is studied. Four different molecular weights of PPO were investigated, to determine how the variation in the polymer coil size affects the Hofmeister effect. The investigation was further conducted for different PPO concentrations, in order to understand the effect of inter-chain interactions on the response to addition of salt. The temperature-driven phase separation of the solutions was monitored by differential scanning calorimetry, which provides the precise value of the phase separation temperature, as well as the enthalpy change accompanied with the transition. It was observed that increasing the molecular weight weakens the effect of the both salts, which is interpreted in terms of a scaling law between the molecular weight and the accessible surface area of the polymers. Increasing the PPO concentration further diminished the NaCl effect, but amplified the NaSCN effect. This difference is attributed to an electrostatic stabilization mechanism in the case of NaSCN.

**General information**

State: Published
Organisations: Department of Chemistry
Authors: Moghaddam, S. Z. (Intern), Thormann, E. (Intern)
Number of pages: 9
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Publication date: 2016
Main Research Area: Technical/natural sciences

**Publication information**

Journal: Journal of Colloid and Interface Science
Volume: 465
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Differential scanning calorimetry, Hofmeister effect, Hydrophobic hydration, Lower critical solution temperature, Poly(propylene oxide)

DOIs:
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Source: FindIt
Hyperpolarised Organic Phosphates as NMR Reporters of Compartmental pH

Organic phosphate metabolites contain functional groups with pKa values near the physiologic pH range, yielding pH-dependent $^{13}$C chemical shift changes of adjacent quaternary carbon sites. When formed in defined cellular compartments from exogenously hyperpolarised $^{13}$C substrates, metabolites thus can yield localised pH values and correlations of organelle pH and catalytic activity.

General information
State: Published
Organisations: Center for Hyperpolarization in Magnetic Resonance, Department of Electrical Engineering, Center for Magnetic Resonance, Department of Chemistry, Organic Chemistry
Authors: Jensen, P. R. (Intern), Meier, S. (Intern)
Number of pages: 4
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Publication date: 2016
Main Research Area: Technical/natural sciences

Publication Information
Journal: Chemical Communications
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BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
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
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
Immunomodulatory N-acyl Dopamine Glycosides from the Icelandic Marine Sponge *Myxilla* incrustans Collected at a Hydrothermal Vent Site

A chemical investigation of the sponge (*Porifera*) *Myxilla* incrustans collected from the unique submarine hydrothermal vent site Strytan, North of Iceland, revealed a novel family of closely related N-acyl dopamine glycosides. Three new compounds, myxillin A (1), B (2) and C (3), were isolated and structurally elucidated using several analytical techniques, such as HR-MS, 1D and 2D NMR spectroscopy. Myxillin A (1) and B (2) were shown to be structurally similar, composed of a dopamine moiety, but differ in the acyl chain length and saturation. The myxillin C (3) has a dehydrotyrosine moiety composing the same acyl chain and glycosylation as myxillin B (2). Myxillins A (1) and C (3) were tested for immunomodulating activity in an in vitro dendritic cell model. Dendritic cells matured and stimulated in the presence of myxillin A (1) secreted lower levels of IL-12p40, whilst dendritic cells matured and stimulated in the presence of myxillin C (3) secreted lower levels of IL-10 compared with dendritic cells matured and stimulated in the presence of the solvent alone. These opposing results indicate that the structural differences in the aromatic ring part of the molecules could have an impact on the immunological effects of dendritic cells. These molecules could, therefore, prove to be important in preventing inflammatory diseases on the one hand, and inducing a response to fight tumors and/or pathogens on the other hand. Further studies will be needed to confirm these potential uses.

**General information**
State: Published
Organisations: Department of Chemistry, Organic Chemistry, University of Iceland, The National University Hospital of Iceland
Authors: Einarsson, T. (Ekstern), Liu, H. B. (Ekstern), Freysdottir, J. (Ekstern), Gofrevsden, C. H. (Intern), Omarsdottir, S. (Ekstern)
Number of pages: 7
Pages: 903-909
Publication date: 2016
Main Research Area: Technical/natural sciences

**Publication information**
Journal: Planta Medica
Volume: 82
Issue number: 9-10
ISSN (Print): 0032-0943
Ratings:
BFI (2018): BFI-level 1
Lignin-carbohydrate complexes (LCCs) are in part responsible for the recalcitrance of lignocellulosics in relation to industrial utilization of biomass for biofuels. Glucuronoyl esterases (GEs) belonging to the carbohydrate esterase family 15 have been proposed to be able to degrade ester LCCs between glucuronic acids in xylans and lignin alcohols. By means of synthesized complex LCC model substrates we provide kinetic data suggesting a preference of fungal GEs for esters of bulky arylalkyl alcohols such as ester LCCs. Furthermore, using natural corn fiber substrate we report the first examples of improved degradation of lignocellulosic biomass by the use of GEs. Improved C5 sugar, glucose and glucuronic acid release was observed when heat pretreated corn fiber was incubated in the presence of GEs from Cerrena unicolor and Trichoderma reesei on top of different commercial cellulase/hemicellulase preparations. These results emphasize the potential of GEs for delignification of biomass thereby improving the overall yield of fermentable sugars for biofuel production.
In-Bead Screening of Hydroxamic Acids for the Identification of HDAC Inhibitors

A one bead–one compound screening format is presented. Following solid-phase synthesis on a photolabile linker, library compounds were readily released and screened inside polymer beads. The release of screening compounds was readily controlled by varying photolysis time and light intensity. Dose-response experiments were carried out to effectively distinguish high- and low-affinity ligands. A library containing 55800 compounds was synthesized and screened in a fluorometric assay, thereby identifying potent HDAC inhibitors with IC\textsubscript{50} values in the nanomolar range.

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry
Authors: Qvortrup, K. (Intern), Nielsen, T. E. (Intern)
Number of pages: 4
Pages: 4548-4551
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Angewandte Chemie
Volume: 128
Issue number: 14
ISSN (Print): 0044-8249
Ratings:
BFI (2018): BFI-level 1
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
In-Bead Screening of Hydroxamic Acids for the Identification of HDAC Inhibitors

A one bead–one compound screening format is presented. Following solid-phase synthesis on a photolabile linker, library compounds were readily released and screened inside polymer beads. The release of screening compounds was readily controlled by varying photolysis time and light intensity. Dose-response experiments were carried out to effectively distinguish high- and low-affinity ligands. A library containing 55,800 compounds was synthesized and screened in a fluorometric assay, thereby identifying potent HDAC inhibitors with IC$_{50}$ values in the nanomolar range.

General information

State: Published
Organisations: Department of Chemistry, Organic Chemistry
Authors: Qvortrup, K. (Intern), Nielsen, T. E. (Intern)
Number of pages: 4
Pages: 4472-4475
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication Information

Volume: 55
Issue number: 14
ISSN (Print): 1433-7851
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
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
Influence of Niche-Specific Nutrients on Secondary Metabolism in Vibrionaceae

Many factors, such as the substrate and the growth phase, influence biosynthesis of secondary metabolites in microorganisms. Therefore, it is crucial to consider these factors when establishing a bioprospecting strategy. Mimicking the conditions of the natural environment has been suggested as a means of inducing or influencing microbial secondary metabolite production. The purpose of the present study was to determine how the bioactivity of Vibrionaceae was influenced by carbon sources typical of their natural environment. We determined how mannose and chitin, compared to glucose, influenced the antibacterial activity of a collection of Vibrionaceae strains isolated because of their ability to produce antibacterial compounds but that in subsequent screenings seemed to have lost this ability. The numbers of bioactive isolates were 2- and 3.5-fold higher when strains were grown on mannose and chitin, respectively, than on glucose. As secondary metabolites are typically produced during late growth, potential producers were also allowed 1 to 2 days of growth before exposure to the pathogen. This strategy led to a 3-fold increase in the number of bioactive strains on glucose and an 8-fold increase on both chitin and mannose. We selected two bioactive strains belonging to species for which antibacterial activity had not previously been identified. Using ultrahigh-performance liquid chromatography-high-resolution mass spectrometry and bioassay-guided fractionation, we found that the siderophore fluvibactin was responsible for the antibacterial activity of Vibrio furnissii and Vibrio fluvialis. These results suggest a role of chitin in the regulation of secondary metabolism in vibrios and demonstrate that considering bacterial ecophysiology during development of screening strategies will facilitate bioprospecting.

General information

State: Published
Organisations: Department of Systems Biology, Novo Nordisk Foundation Center for Biosustainability, Bacterial Ecophysiology and Biotechnology, Department of Chemistry, Organic Chemistry, Metabolomics Platform
Authors: Giubergia, S. (intern), Phippen, C. (intern), Gotfredsen, C. H. (intern), Nielsen, K. F. (intern), Gram, L. (intern)
Number of pages: 10
Pages: 4035-4044
Publication date: 2016
The stability of cyclic peptide assemblies (CPs) forming a macromolecular nanotube structure was investigated in solvents of different polarity using computational methods. The stability and structure of the complexes were studied using traditional molecular dynamics (MD). Energy of dissociation was estimated from steered MD in combination with umbrella sampling simulations. A cyclic peptide nanotube (CPNT) was constructed by stacking of eight cyclo[(d-Trp-l-Gln-d-Trp-l-Glu)2], and hereafter is referred to as (WQWE)8. Its dissociation was studied by pulling 1, 2, or 3 subunits from the nanotube. The crucial point in the dissociation event of the CP subunit(s) is the breaking of backbone–backbone hydrogen bonds and consecutive annihilation of side chain interactions. Gibbs free energy calculations to estimate the binding affinity of CP subunit(s) reveal that the (WQWE)8 nanotube is significantly more stable in non-polar environments than in polar environments. The presently investigated nanotube, (WQWE)8, displays a higher stability in polar solvent than the previously studied nanotube, (QAEA)8. It appears that tryptophan contributes favorable to the improved stability by forming side chain–side chain hydrogen bonds.
In-situ construction of three-dimensional titania network on Ti foil toward enhanced performance of flexible dye-sensitized solar cells

Three-dimensional titania network was in-situ constructed on Ti foil via sequential acid and hydrogen peroxide treatments. The titania network was pure anatase phase and homogeneously covered on the titanium grain surface, which largely enhanced the roughness of the Ti foil. The as-received Ti foil and the treated one were used as the flexible substrates of DSSCs, and energy conversion efficiencies of 3.74% and 4.98% were obtained, respectively. Such remarkable increment can be ascribed to the good electrical contact between the nanocrystalline TiO2 and the Ti foil, the improved electron percolation pathways and recombination inhibition of electrons in Ti substrate with triiodide ions in electrolyte. Flexible DSSCs based on the treated Ti foil showed relatively good mechanical stability, which exhibited 97.3% retention of the initial efficiency after twenty consecutive bending.

General information

State: Published
Organisations: Department of Chemistry, NanoChemistry, Organic Chemistry, Donghua University
Authors: Rui, Y. (Ekstern), Wang, Y. (Ekstern), Zhang, Q. (Ekstern), Chi, Q. (Intern), Zhang, M. (Intern), Wang, H. (Ekstern), Li, Y. (Ekstern), Hou, C. (Intern)
Number of pages: 8
Pages: 210-217
Publication date: 2016
Conference: 10th International Conference on Surfaces, Coatings and Nanostructured Materials (NANOSMAT-10), Manchester, United Kingdom, 13/09/2015 - 13/09/2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Applied Surface Science
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Ratings:
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.37 SJR 0.951 SNIP 1.225
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.914 SNIP 1.3 CiteScore 3.13
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.958 SNIP 1.477 CiteScore 2.96
Web of Science (2014): Indexed yes
Investigating the Sensitivity of NAD⁺-dependent Sirtuin Deacylation Activities to NADH

Protein lysine posttranslational modification by an increasing number of different acyl groups is becoming appreciated as a regulatory mechanism in cellular biology. Sirtuins are class III histone deacylases that use NAD⁺ as a co-substrate during amide bond hydrolysis. Several studies have described the sirtuins as sensors of the NAD⁺/NADH ratio, but it has not been formally tested for all the mammalian sirtuins in vitro. To address this problem, we first synthesized a wide variety of peptide-based probes, which were used to identify the range of hydrolytic activities of human sirtuins. These probes included aliphatic -N-acyllysine modifications with hydrocarbon lengths ranging from formyl (C₁) to palmitoyl (C₁₆) as well as negatively charged dicarboxyl-derived modifications. In addition to the well established activities of the sirtuins, "long chain" acyllysine modifications were also shown to be prone to hydrolytic cleavage by SIRT1-3 and SIRT6, supporting recent findings. We then tested the ability of NADH, ADP-ribose, and nicotinamide to inhibit these NAD⁺-dependent deacylation activities of the sirtuins. In the commonly used 7-amino-4-methylcoumarin-coupled fluorescence-based assay, the fluorophore has significant spectral overlap with NADH and therefore cannot be used to measure inhibition by NADH. Therefore, we turned to an HPLC-MS-based assay to directly monitor the conversion of acylated peptides to their deacylated forms. All tested sirtuin deacylase activities showed sensitivity to NADH in this assay. However, the inhibitory concentrations of NADH in these assays are far greater than the predicted concentrations of NADH in cells; therefore, our
data indicate that NADH is unlikely to inhibit sirtuins in vivo. These data suggest a re-evaluation of the sirtuins as direct sensors of the NAD\(^+/\)NADH ratio.

**General information**

**State:** Published  
**Organisations:** Department of Chemistry, Organic Chemistry, Duke University, University of Copenhagen, University of Colorado  
**Number of pages:** 14  
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**Main Research Area:** Technical/natural sciences

**Publication information**

**Journal:** Journal of Biological Chemistry  
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BFI (2017): BFI-level 2  
Web of Science (2017): Indexed yes  
BFI (2016): BFI-level 2  
Scopus rating (2016): CiteScore 4.17 SJR 2.755 SNIP 1.125  
Web of Science (2016): Indexed yes  
BFI (2015): BFI-level 2  
Scopus rating (2015): SJR 3.121 SNIP 1.184 CiteScore 4.4  
Web of Science (2015): Indexed yes  
BFI (2014): BFI-level 2  
Scopus rating (2014): SJR 3.254 SNIP 1.222 CiteScore 4.5  
Web of Science (2014): Indexed yes  
BFI (2013): BFI-level 2  
Scopus rating (2013): SJR 3.369 SNIP 1.231 CiteScore 4.87  
ISI indexed (2013): ISI indexed yes  
Web of Science (2013): Indexed yes  
BFI (2012): BFI-level 2  
Scopus rating (2012): SJR 3.361 SNIP 1.244 CiteScore 4.97  
ISI indexed (2012): ISI indexed yes  
Web of Science (2012): Indexed yes  
BFI (2011): BFI-level 2  
Scopus rating (2011): SJR 3.495 SNIP 1.26 CiteScore 4.97  
ISI indexed (2011): ISI indexed yes  
Web of Science (2011): Indexed yes  
BFI (2010): BFI-level 2  
Scopus rating (2010): SJR 3.923 SNIP 1.342  
Web of Science (2010): Indexed yes  
BFI (2009): BFI-level 2  
Scopus rating (2009): SJR 4.158 SNIP 1.344  
Web of Science (2009): Indexed yes  
BFI (2008): BFI-level 2  
Scopus rating (2008): SJR 4.289 SNIP 1.375  
Web of Science (2008): Indexed yes  
Scopus rating (2007): SJR 4.277 SNIP 1.373  
Web of Science (2007): Indexed yes
Compounds wettability is critical for a number of central processes including disintegration, dispersion, solubilisation and dissolution. It is therefore an important optimisation parameter both in drug discovery but also as guidance for formulation selection and optimisation. Wettability for a compound is determined by its contact angle to a liquid, which in the present study was measured using the sessile drop method applied to a disc compact of the compound. Precise determination of the contact angle is important should it be used to either rank compounds or selected excipients to e.g. increase the wetting from a solid dosage form. Since surface roughness of the compact has been suggested to influence the measurement this study investigated if the surface quality, in terms of surface porosity, had an influence on the measured contact angle. A correlation to surface porosity was observed, however for six out of seven compounds similar results were obtained by applying a standard pressure (866MPa) to the discs in their preparation. The data presented in the present work therefore suggest that a constant high pressure should be sufficient for most compounds when determining the contact angle. Only for special cases where compounds have poor compressibility would there be a need for a surface-quality-control step before the contact angle determination.
Investigations of beer carbohydrates with increased 13C sensitivity

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry, Aarhus University
In vivo Evaluation of PEGylated $^{64}$Cu-liposomes with Theranostic and Radiotherapeutic Potential using Micro PET/CT

The objective of this study was to evaluate the potential of PEGylated $^{64}$Cu-liposomes in clinical diagnostic positron emission tomography (PET) imaging and PEGylated $^{177}$Lu-liposomes in internal tumor radiotherapy through in vivo characterization and dosimetric analysis in a human xenograft mouse model. Liposomes with 5 and 10 mol% PEG were characterized with respect to size, charge, and $^{64}$Cu- and $^{177}$Lu-loading efficiency. The tumor imaging potential of $^{64}$Cu-loaded liposomes was evaluated in terms of in vivo biodistribution, tumor accumulation and tumor-to-muscle (T/M) ratios, using PET imaging. The potential of PEGylated liposomes for diagnostic and therapeutic applications was further evaluated through dosimetry analysis using OLINDA/EXM software. The $^{64}$Cu-liposomes were used as biological surrogates to estimate the organ and tumor kinetics of $^{177}$Lu-liposomes. High remote loading efficiency (>95%) was obtained for both $^{64}$Cu and $^{177}$Lu radioisotopes with PEGylated liposomes, and essentially no leakage of the encapsulated radionuclides was observed upon storage and after serum incubation for 24 h at 37 °C. The 10 mol% PEG liposomes showed higher tumor accumulation (6.2±0.2 %ID/g) than the 5 mol% PEG liposomes, as evaluated by PET imaging. Thedosimetry analysis of the $^{64}$Cu-liposomes estimated an acceptable total effective dose of 3.3·10⁻² mSv/MBq for diagnostic imaging in patients. A high absorbed tumor dose (114 mGy/MBq) was estimated for the potential radiotherapeutic $^{177}$Lu-liposomes. The overall preclinical profile of PEGylated $^{64}$Cu-liposomes showed high potential as a new PET theranostic tracer for imaging in humans. Dosimetry results predicted that initial administered activity of 200 MBq of $^{64}$Cu-liposomes should be acceptable in patients. Work is in progress to validate the utility of PEGylated $^{64}$Cu-liposomes in a clinical research programme. The high absorbed tumor dose (114 mGy/MBq) estimated for $^{177}$Lu-liposomes and the preliminary dosimetric studies justify further therapeutic and dosimetry investigation of $^{177}$Lu-liposomes in animals before potential testing in man.

General information

State: Published
Organisations: Department of Micro- and Nanotechnology, Colloids and Biological Interfaces, Center for Nanomedicine and Theranostics, Department of Chemistry, Center for Nuclear Technologies, The Hevesy Laboratory, University of Copenhagen
Authors: Petersen, A. L. (Intern), Henriksen, J. R. (Intern), Binderup, T. (Ekstern), Elema, D. R. (Intern), Rasmussen, P. H. (Intern), Hag, A. M. (Ekstern), Kjaer, A. (Ekstern), Andresen, T. L. (Intern)
Number of pages: 12
Pages: 941-952
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: European Journal of Nuclear Medicine and Molecular Imaging
Volume: 43
Issue number: 5
ISSN (Print): 1619-7070
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.84 SJR 2.396 SNIP 1.898
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 2.066 SNIP 1.633 CiteScore 3.94
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.008 SNIP 1.76 CiteScore 4.19
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.007 SNIP 1.749 CiteScore 4.17
ISI indexed (2013): ISI indexed yes
Graphene based nanomaterials have been a hot topic since 2004. These materials have shown some notable advantages, including large surface areas, high flexibility and reasonably good conductivity and mechanical strength, suitable for a wide range of electrochemical applications from sensors to energy technologies. In this presentation, we have explored the combination of redox active Prussian Blue (PB) nanostructures (e.g., core-shell Gold@Prussian Blue (Au@PB) nanoparticles (NPs) and interlocked PB nanocubes) with chemically exfoliated graphene to prepare multifunctional composites as electrochemical catalysts and supercapacitor electrode materials. Those nanocomposites were systematically characterized by AFM, SEM, TEM and XPS. The results confirmed all PB nanostructures were well combined with graphene nanosheets. Furthermore, PB nanostructure functionalized graphene materials were fabricated into disposable paper sensors and supercapacitor electrodes. For example, Au@PBNPs hybrid graphenoxde suspension was filtered via layer-by-layer into functional GO paper, which was further converted into electrically conductive reduced GO (RGO)/Au@PB paper via hydrazine vapour reduction. The whole procedure is outlined schematically in Fig. 1. Resulting sandwich functionalized graphene papers have sufficient conductivity and flexibility, and robust mechanical strength, which can be cut into freestanding electrodes. Such electrodes with the advantages of low cost and scalable production capacity, for example used as non-enzymatic electrochemical sensors, are of particular interest in the areas of flexible, disposable, simple and low-cost sensors.

**Prussian Blue Modified Graphene Enable Multifunctional Electrochemical Application**

Graphene based nanomaterials have been a hot topic since 2004. These materials have shown some notable advantages, including large surface areas, high flexibility and reasonably good conductivity and mechanical strength, suitable for a wide range of electrochemical applications from sensors to energy technologies. In this presentation, we have explored the combination of redox active Prussian Blue (PB) nanostructures (e.g., core-shell Gold@Prussian Blue (Au@PB) nanoparticles (NPs) and interlocked PB nanocubes) with chemically exfoliated graphene to prepare multifunctional composites as electrochemical catalysts and supercapacitor electrode materials. Those nanocomposites were systematically characterized by AFM, SEM, TEM and XPS. The results confirmed all PB nanostructures were well combined with graphene nanosheets. Furthermore, PB nanostructure functionalized graphene materials were fabricated into disposable paper sensors and supercapacitor electrodes. For example, Au@PBNPs hybrid graphene oxide suspension was filtered via layer-by-layer into functional GO paper, which was further converted into electrically conductive reduced GO (RGO)/Au@PB paper via hydrazine vapour reduction. The whole process is outlined schematically in Fig. 1. Resulting sandwich functionalized graphene papers have sufficient conductivity and flexibility, and robust mechanical strength, which can be cut into freestanding electrodes. Such electrodes with the advantages of low cost and scalable production capacity, for example used as non-enzymatic electrochemical sensors, are of particular interest in the areas of flexible, disposable, simple and low-cost sensors.

**General information**

State: Published
Organisations: Department of Chemistry, NanoChemistry, Organic Chemistry
Authors: Zhang, M. (Intern), Halder, A. (Intern), Hou, C. (Intern), Chi, Q. (Intern)
Number of pages: 1
Publication date: 2016
Iridoids in Hydrangeaceae

The content of glycosides in *Kirengeshoma palmata* and *Jamesia americana* (Hydrangeaceae) have been investigated. The former contains loganin and secoiridoids, including the alkaloid demethylalangiside. The latter contains no iridoids, but the known glucosides arbutin, picein and prunasin. In order to further investigate the chemotaxonomy of the family Hydrangeaceae, the distribution of the iridoid and secoiridoid glucosides as well as the known biosynthetic pathways to these compounds have been reviewed. However, only a few genera of the family has been investigated. Loganin, secolloganin, and derivatives of these are common. The genus *Deutzia* is characteristic in containing more structurally simple iridoids in which C-10 has been lost during biosynthesis. Such compounds have so far only been reported from the genus *Mentzelia* (Loasaceae). The taxonomic relationships between Hydrangeaceae and the closely related Cornaceae and Loasaceae is discussed and found to agree well with recent DNA sequence results.
Laccase-3D graphene as catalysts for oxygen reduction in biocathodes

**General information**
- **State**: Published
- **Organisations**: Department of Chemistry, NanoChemistry, Organic Chemistry
- **Authors**: Shen, F. (Intern), Werchmeister, R. M. L. (Intern), Ulstrup, J. (Intern), Zhang, J. (Intern)
- **Number of pages**: 1
- **Publication date**: 2016
- **Main Research Area**: Technical/natural sciences
- **Links**: [http://www.sustain.dtu.dk/](http://www.sustain.dtu.dk/)

**Bibliographical note**
- Sustain Abstract I-9
- **Publication**: Research - peer-review › Conference abstract for conference – Annual report year: 2016

**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
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Organisations: Organic Chemistry, Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Authors: Melián Rodríguez, M. (Intern), Riisager, A. (Intern), Kegnæs, S. (Intern), Shunmugavel, S. (Intern)
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Loss of stability and hydrophobicity of presenilin 1 mutations causing Alzheimer’s Disease
Nearly 200 mutations in the gene coding for presenilin 1 (PSEN1) cause early-onset Alzheimer’s Disease, yet the molecular mechanism remains obscure. As a meta-analysis, we compiled available clinical and biochemical data for PSEN1 variants and correlated these to chemical properties of the mutants. We found statistically significant relationships between relative Aβ42 levels and clinical age of onset. We then computed chemical properties of the mutants from a variety of computational chemistry tools. Relative Aβ42 levels correlated significantly (95% confidence or more from p-values of linear regression) with loss of hydrophobicity for four different regression analyses (squared correlation coefficient of linear regression $R^2$ of 0.41–0.51) and with increased polarity ($R^2 = 0.47$, 0.59) and loss of protein stability ($R^2 = 0.39$, 0.63) for two independent data sets. Age of onset of patients carrying PSEN1 variants correlated with increased polarity ($R^2 = 0.49$, 0.40) and loss of stability ($R^2 = 0.75$, 0.44) of the protein for both data sets. These relations suggest that mutants impair the membrane-associated structural integrity of presenilin by reducing hydrophobic membrane association and overall protein stability. This explains why the many mutations that spread out across the protein and far from the catalytic aspartates can cause disease. The identified molecular determinants of clinical age of symptom onset may be relevant to future presenilin-modulating therapies specifically directed towards increasing the structural integrity and packing of the protein.

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Organisations: Department of Chemistry
LOX1 inhibition with small molecules
Lipoxygenases (LOXs) are nonheme, iron-containing dioxygenases that catalyze the dioxygenation of polyunsaturated fatty acids and are widely distributed among plant and animal species. Human LOXs, now identified as key enzymes in the pathogenesis of major disorders, have increasingly drawn the attention as targets and great effort has been made for the discovery and design of suitable inhibitors, to which end both pharmacological and computational methods have been employed. In the present work, using pharmacophore modeling and docking, we attempt to elucidate the inhibition of LOX1 with a new inhibitor, albidoside, an iridoid glucoside isolated from plants of the Scutellaria genus. Through a pharmacophore approach, complementarities between the ligand and the binding site are explored and a plausible mode of binding with the protein is suggested for albidoside.

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Organisations: Organic Chemistry, Department of Chemistry, Department of Systems Biology, Center for Biological Sequence Analysis
Authors: Gousiadou, C. (Intern), Kouskoumvekaki, I. (Intern)
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Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.474 SNIP 0.673 CiteScore 1.87
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.599 SNIP 0.702 CiteScore 1.9
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.574 SNIP 0.783 CiteScore 2.23
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.746 SNIP 0.869 CiteScore 2.28
ISI indexed (2012): ISI indexed yes
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BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.637 SNIP 0.843 CiteScore 2.21
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.681 SNIP 0.891
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.642 SNIP 0.889
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.815 SNIP 0.829
Scopus rating (2007): SJR 0.804 SNIP 0.762
Scopus rating (2006): SJR 0.71 SNIP 0.877
Scopus rating (2005): SJR 0.936 SNIP 1.076
Mechanism and Stereoselectivity of Zeolite-catalysed Sugar Isomerisation in Alcohols

Glucose isomerisation to fructose can occur by different pathways and the mechanism of zeolite-catalysed glucose isomerisation in methanol has remained incompletely understood. Herein, the mechanism is studied using an 1H-13C HSQC NMR assay resolving different fructose isotopomers. We find that zeolite-catalysed glucose isomerisation proceeds predominantly via a hydride shift into the pro-R position of fructose, thus resembling the stereoselectivity of the enzymatic isomerisation process.

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Organisations: Organic Chemistry, Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Haldor Topsoe AS
Authors: Shunmugavel, S. (Intern), Riisager, A. (Intern), Taarning, E. (Ekstern), Meier, S. (Intern)
Number of pages: 4
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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
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Mechanistic Investigation of Molybdate-Catalysed Transfer Hydrodeoxygenation

The molybdate-catalysed transfer hydrodeoxygenation (HDO) of benzyl alcohol to toluene driven by oxidation of the solvent isopropyl alcohol to acetone has been investigated by using a combination of experimental and computational methods. A Hammett study that compared the relative rates for the transfer HDO of five para-substituted benzylic alcohols was carried out. Density-functional theory (DFT) calculations suggest a transition state with significant loss of aromaticity contributes to the lack of linearity observed in the Hammett study. The transfer HDO could also be carried out in neat PhCH₂OH at 175°C. Under these conditions, PhCH₂OH underwent disproportionation to yield benzaldehyde, toluene, and significant amounts of bibenzyl. Isotopic-labelling experiments (using PhCH₂OD and PhCD₂OH) showed that incorporation of deuterium into the resultant toluene originated from the αposition of benzyl alcohol, which is in line with the mechanism suggested by the DFT study.

General information
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Organisations: Department of Chemistry, Organic Chemistry
Authors: Larsen, D. B. (Intern), Petersen, A. R. (Intern), Dethlefsen, J. R. (Intern), Gorfo, A. T. (Intern), Fristrup, P. (Intern)
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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.

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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)
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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
Method Development in the Regioselective Glycosylation of Unprotected Carbohydrates

Project 1: Tin-mediated glycosylation of unprotected hexopyranosides
The regioselective glycosylation at the 6 position in 2,3,4,6-unprotected hexopyranosides has been investigated with dibutyltin oxide as the directing agent. Perbenzylated hexopyranosyl bromides were employed as the donors and the glycosylations were promoted by tetrabutylammonium bromide. The couplings were completely selective and gave rise to a number of 1,6-linked disaccharides with 1,2- cis-linked orientation.

Project 2: Boron-mediated glycosylation of unprotected carbohydrates
Boron-mediated regioselective Koenigs-Knorr glycosylation has been studied with unprotected acceptors. By means of organoboron derivatives, cis-diols in acceptors can be either activated or masked via an ester formation.

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Organisations: Department of Chemistry, Organic Chemistry
Authors: Niedbal, D. A. (Intern), Madsen, R. (Intern)
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Methoxycarbonylation of alkenes with biomass-derived CO
The production of chemicals, fuels and energy from renewable feedstock, such as biomass, has seen increasing interest in the last decade. One of the key issues regarding biorenewables is the reduction of the oxygenation grade in molecules, the removal of oxygen. This thesis focuses on the removal of oxygen, in the form of carbon monoxide, and use in a tandem reaction for the methoxycarbonylation of alkenes. Furthermore, the production of γ-valerolactone (GVL), a
promising green fuel has been exploited. Chapter 1: Introduction provides a walk-through of subjects like biomass and its utility, dehydration of sugars, the importance of the furanoic platform and carbonylation reactions. All these arguments are described in detail, taking into account the current and past research, accurately chosen in order to offer an insight for next chapters. Chapter 2: Experimental, deals with the analytical techniques and the catalytic setups of the reactions. Chapter 3: Results and Discussion, is divided into two main parts. The first one reports and discuss the data obtained after the methoxycarbonylation reaction of 5 HMF (5-hydroxymethyl furfural), to yield methyl heptanoate (MH), methyl levulate (ML), and GVL, the three products we investigated. The catalytic system is optimized, following the indication given by the results of the reactions. All the steps of the process are deeply discussed in this section. Consideration on the reaction time, on the choice and the quantity of the acidic catalyst, the nature and the amount of the palladium precursor and the phosphine ligand, a screening of the reaction temperatures, and an investigation regarding different substrates (with a furanic backbone), alkenes and alcohols have been done. Our catalytic system proved to be valid to give good yields in a one-pot reaction from HMF to valuable products. All the data are gathered after GC-FID, GS-MS and HPLC analysis, run using naphthalene as internal standard. The second part examines the methoxycarbonylation reaction applied to different carbohydrates. Insights on the kinetics of the reaction and the reactivity of various carbohydrates can be inferred from the analysis of the reported data. Through this screening, our catalytic system proved to be active on a broad range sugars, from monosaccharides to polysaccharides, such as inulin and starch. Chapter 4: Conclusions, it summarizes the results, future perspectives and possible developments.
Molecular Assembly of Hemin on Single-Crystal Au(111)-electrode Surfaces

Iron porphyrin, hemin, is the active core in cytochromes, haemoglobin and myoglobin, and enzymes such as the peroxidases. These metalloproteins are engaged in respiratory electron transfer, oxygen transport and storage, and enzyme catalysis in the biosynthesis of a range of metabolites. Hemin itself also acts as catalyst in electrochemical reduction of dioxygen and other small inert molecules such as nitrogen monoxide, and in electrochemiluminescent detection of dioxygen, peroxide, DNA, and proteins. π-π interactions of hemin with carbon materials have been broadly
studied. Hemin on noble metal surfaces has been prime targets in high-resolution STM but much less used in applied contexts such as biosensors and drug delivery. How hemin molecules interact with noble metal surfaces offers, however, other challenges in nanoscale and single-molecule science. We have studied hemin adsorption on well-defined single-crystal Au(111)-electrodesurfaces using electrochemistry combined with scanning tunnelling microscopy under electrochemical control. Hemin gives two voltammetric peaks assigned to adsorbed monomers and dimmers (Fig. 1A). In situ STM shows that hemin self-assembles in ordered monolayers through non-covalent adsorption, as the reconstruction of the Au-(111) surface underneath the hemin layer is clearly visible (Fig. 1B).

Molecular Basis of Enhanced Activity in Factor VIIa-Trypsin Variants Conveys Insights into Tissue Factor-mediated Allosteric Regulation of Factor VIIa Activity

The complex of coagulation factor VIIa (FVIIa), a trypsin-like serine protease, and membrane-bound tissue factor (TF) initiates blood coagulation upon vascular injury. Binding of TF to FVIIa promotes allosteric conformational changes in the FVIIa protease domain and improves its catalytic properties. Extensive studies have revealed two putative pathways for this allosteric communication. Here we provide further details of this allosteric communication by investigating FVIIa loop swap variants containing the 170 loop of trypsin that display TF-independent enhanced activity. Using x-ray crystallography, we show that the introduced 170 loop from trypsin directly interacts with the FVIIa active site, stabilizing segment 215-217 and activation loop 3, leading to enhanced activity. Molecular dynamics simulations and novel fluorescence quenching studies support that segment 215-217 conformation is pivotal to the enhanced activity of the FVIIa variants. We speculate that the allosteric regulation of FVIIa activity by TF binding follows a similar path in conjunction with protease domain N terminus insertion, suggesting a more complete molecular basis of TF-mediated allosteric enhancement of FVIIa activity.
New Concepts of Quality Assurance in Analytical Chemistry: Will They Influence the Way We Conduct Science in General?

According to the guide Vocabulary in Metrology (VIM3) (JCGM, 2008), the definition of the concepts of trueness and accuracy has been revised, which has an important impact on analytical chemistry. Additionally, Eurachem/CITAC has...
published a new edition of the guide to Quantifying Uncertainty in Analytical Measurement (QUAM) (CITAC and Eurachem, 2012). These two documents, together, form a new basis for the evaluation of data. Results of prominent technologies of inductively coupled plasma mass spectrometry (ICP-MS), for determination of chloride-isotope ratios (35 Cl/37 Cl) and inductively coupled plasma optical emission spectrometry (ICP-OES) for determination of sodium, were evaluated in terms of the true level of uncertainty and revealed a genuine problem for science that was not addressed in VIM3 and QUAM. Comparison of theory and experimentation definitely requires statistical tools, but in contemporary science two approaches to the implementation of statistics in decision making are used: 1. Short-term precision and 2. long-term precision. Both approaches are valid and both are described using the same methods of statistics. However, they lead to completely different conclusions and decisions. Despite good intentions and new concepts, as well as practices and procedures for quality assurance, it is shown by these two examples that these efforts may be inadequate or mislead scientists into making major mistakes in the decision-making process. A set of equations is supplied, which are based on the propagation of uncertainty, and the implication of results and conclusions for other fields of science is discussed.

**General information**

State: Published
Organisations: Analytical Chemistry, Department of Chemistry, Organic Chemistry, Molenaar Geoconsulting, Botswana International University of Science and Technology
Authors: Andersen, J. (Intern), Glasdam, S. (Intern), Larsen, D. B. (Intern), Molenaar, N. (Ekstern)
Number of pages: 9
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- Web of Science (2017): Indexed Yes
- BFI (2016): BFI-level 1
- Scopus rating (2016): CiteScore 1.28 SJR 0.338 SNIP 0.803
- Web of Science (2016): Indexed yes
- BFI (2015): BFI-level 1
- Scopus rating (2015): SJR 0.383 SNIP 0.829 CiteScore 1.28
- BFI (2014): BFI-level 1
- Scopus rating (2014): SJR 0.404 SNIP 0.791 CiteScore 1.2
- BFI (2013): BFI-level 1
- Scopus rating (2013): SJR 0.411 SNIP 0.729 CiteScore 1.05
- ISI indexed (2013): ISI indexed yes
- BFI (2012): BFI-level 1
- Scopus rating (2012): SJR 0.404 SNIP 0.813 CiteScore 1.15
- ISI indexed (2012): ISI indexed yes
- BFI (2011): BFI-level 1
- Scopus rating (2011): SJR 0.421 SNIP 0.646 CiteScore 1.01
- ISI indexed (2011): ISI indexed yes
- BFI (2010): BFI-level 1
- Scopus rating (2010): SJR 0.423 SNIP 0.566
- BFI (2009): BFI-level 1
- Scopus rating (2009): SJR 0.337 SNIP 0.519
- BFI (2008): BFI-level 1
- Scopus rating (2008): SJR 0.369 SNIP 0.535
- Scopus rating (2007): SJR 0.313 SNIP 0.365
Non-resonant dynamic stark control of vibrational motion with optimized laser pulses
The term dynamic Stark control (DSC) has been used to describe methods of quantum control related to the dynamic Stark effect, i.e., a time-dependent distortion of energy levels. Here, we employ analytical models that present clear and concise interpretations of the principles behind DSC. Within a linearly forced harmonic oscillator model of vibrational excitation, we show how the vibrational amplitude is related to the pulse envelope, and independent of the carrier frequency of the laser pulse, in the DSC regime. Furthermore, we shed light on the DSC regarding the construction of optimal pulse envelopes - from a time-domain as well as a frequency-domain perspective. Finally, in a numerical study beyond the linearly forced harmonic oscillator model, we show that a pulse envelope can be constructed such that a vibrational excitation into a specific excited vibrational eigenstate is accomplished. The pulse envelope is constructed such that high intensities are avoided in order to eliminate the process of ionization.

General information
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Organisations: Department of Chemistry, Department of Micro- and Nanotechnology
Authors: Thomas, E. F. (Intern), Henriksen, N. E. (Intern)
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Scopus rating (2016): CiteScore 2.13 SJR 1.073 SNIP 0.755
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.953 SNIP 0.767 CiteScore 1.98
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.386 SNIP 0.989 CiteScore 2.54
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Novel α-L-Fucosidases from a Soil Metagenome for Production of Fucosylated Human Milk Oligosaccharides

This paper describes the discovery of novel α-L-fucosidases and evaluation of their potential to catalyse the transglycosylation reaction leading to production of fucosylated human milk oligosaccharides. Seven novel α-L-fucosidase-encoding genes were identified by functional screening of a soil-derived metagenome library and expressed in *E. coli* as recombinant 6xHis-tagged proteins. All seven fucosidases belong to glycosyl hydrolase family 29 (GH 29). Six of the seven α-L-fucosidases were substrate-inhibited, moderately thermostable and most hydrolytically active in the pH range 6-7, when tested with para-nitrophenyl-α-L-fucopyranoside (pNP-Fuc) as the substrate. In contrast, one fucosidase (Mfuc6) exhibited a high pH optimum and an unusual sigmoidal kinetics towards pNP-Fuc substrate. When tested for trans-fucosylation activity using pNP-Fuc as donor, most of the enzymes were able to transfer fucose to pNP-Fuc (self-
condensation) or to lactose. With the α-L-fucosidase from *Thermotoga maritima* and the metagenome-derived Mfuc5, different fucosyllactose variants including the principal fucosylated HMO 2'-fucosyllactose were synthesised in yields of up to ~6.4%. Mfuc5 was able to release fucose from xyloglucan and could also use it as a fucosyl-donor for synthesis of fucosyllactose. This is the first study describing the use of glycosyl hydrolases for the synthesis of genuine fucosylated human milk oligosaccharides.

**General information**
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Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, Department of Chemistry, Organic Chemistry, University of Copenhagen
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Scopus rating (2016): CiteScore 3.11 SJR 1.201 SNIP 1.092
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.414 SNIP 1.131 CiteScore 3.32
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.545 SNIP 1.141 CiteScore 3.54
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.74 SNIP 1.147 CiteScore 3.94
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.945 SNIP 1.142 CiteScore 4.15
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Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.369 SNIP 1.23 CiteScore 4.58
ISI indexed (2011): ISI indexed no
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 2.631 SNIP 1.161
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 2.473 SNIP 0.985
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 2.323 SNIP 0.96
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.289 SNIP 0.525
Observations on the Influence of Precursor Conformations on Macrocyclization Reactions

Macrocycles hold great promise in drug discovery as an underutilized class of lead compounds. The low abundance of these molecules can, in part, be explained by the inherent difficulties in the synthesis of macrocycles and the lack of general methods for their rapid assembly. We have undertaken a research program aimed at developing methods for facile synthesis of macrocycles from simple precursors. The synthesis of two new cyclization precursors is described and the results of their reaction with thionyl chloride are presented and discussed. Whereas one acyclic diol smoothly underwent macrolization to afford a mixture of diastereomeric sulfites, subjection of the other precursor to identical reaction conditions resulted in the isolation of the linear dichloride. We hypothesize that there is a difference in the ability of the two molecules to adopt a conformation that is germane to macrolization, a proposition that is supported by conformational analyses using molecular mechanics.

General information
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Organisations: Organic Chemistry, Department of Chemistry, Technical University of Denmark
Authors: Hammershøj, P. (Intern), Beldring, K. (Eksterm), Nielsen, A. R. (Eksterm), Fristrup, P. (Intern), Clausen, M. H. (Intern)
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Scopus rating (2016): CiteScore 2.74 SJR 1.133 SNIP 0.653
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.198 SNIP 0.758 CiteScore 2.88
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.181 SNIP 0.767 CiteScore 2.96
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.292 SNIP 0.796 CiteScore 2.96
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Observing Solvation Dynamics with Simultaneous Femtosecond X-ray Emission Spectroscopy and X-ray Scattering

In liquid phase chemistry dynamic solute solvent interactions often govern the path, ultimate outcome, and efficiency of chemical reactions. These steps involve many-body movements on subpicosecond time scales and thus ultrafast structural tools capable of capturing both intramolecular electronic and structural changes, and local solvent structural changes are desired. We have studied the intra- and intermolecular dynamics of a model chromophore, aqueous \([\text{Fe(bpy)}_3]^2+\), with complementary X-ray tools in a single experiment exploiting intense XFEL radiation as a probe. We monitored the ultrafast structural rearrangement of the solute with X-ray emission spectroscopy, thus establishing time zero for the ensuing X-ray diffuse scattering analysis. The simultaneously recorded X-ray diffuse scattering attens reveal slower subpicosecond dynamics triggered by the intramolecular structural dynamics of the photoexcited solute. By simultaneous combination of both methods only, we can extract new information about the solvation dynamic processes unfolding during the first picosecond (ps). The measured bulk solvent density increase of 0.2% indicates a dramatic change of the solvation shell around each photoexcited solute, confirming previous ab initio molecular dynamics simulations. Structural changes in the aqueous solvent associated with density and temperature changes occur with similar to 1 ps time constants, characteristic for structural dynamics in water. This slower time scale of the solvent response allows us to directly observe the structure of the excited solute molecules well before the solvent contributions become dominant.
On the Carbon Solubility in Expanded Austenite and Formation of Hägg Carbide in AISI 316 Stainless Steel

The carbon solubility in expanded austenite is investigated by controlled low temperature gaseous through-carburizing of AISI 316 stainless steel thin foils with thermogravimetry and synchrotron powder diffraction analysis. Carburizing is carried out in C2H2–H2–N2 and CO–H2–N2 atmospheres at 380–420 °C and 465–470 °C, respectively. Hägg carbide (\(x-M_5C_2\)) develops when the carbon content in the expanded austenite exceeds the metastable solubility limit; the transformation of carbon expanded austenite into Hägg carbide occurs irrespective of carburizing temperature in the investigated temperature range (380–470 °C). The maximum solubility of carbon in expanded austenite (380 °C) is found to correspond to an occupancy (\(y_C\)) of 0.220 of the interstitial octahedral sites of the austenite lattice (i.e., 4.74wt% C). Decomposition of Hägg carbide into \(M_7C_3\) occurs upon prolonged carburizing treatment or thermal exposure in inert atmosphere (in situ synchrotron experiments).

General information
State: Published
Organisations: Department of Mechanical Engineering, Materials and Surface Engineering, Department of Chemistry, X-ray Crystallography
Authors: Christiansen, T. L. (Intern), Ståhl, K. (Intern), Brink, B. (Intern), Somers, M. A. J. (Intern)
Number of pages: 11
Pages: 1385–1405
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Steel Research International
Volume: 87
Issue number: 11
ISSN (Print): 1611-3683
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.24 SJR 0.665 SNIP 1.013
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.479 SNIP 0.713 CiteScore 0.74
BFI (2014): BFI-level 1
Oxidation of lignin in hemp fibres by laccase: effects on mechanical properties of hemp fibres and unidirectional fibre/epoxy composites

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, The Danish Polymer Centre, Department of Chemistry, Organic Chemistry, University of Hamburg
Authors: Liu, M. (Intern), Baum, A. (Intern), Odermatt, J. (Ekstern), Berger, J. (Ekstern), Yu, L. (Intern), Zeuner, B. (Intern), Thygesen, A. (Intern), Holck, J. (Intern), Meyer, A. S. (Intern)
Number of pages: 1
Publication date: 2016
Main Research Area: Technical/natural sciences
Links:
http://www.sustain.dtu.dk/

Bibliographical note
Sustain Abstract M-19
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2016
Phase-only laser control in the weak-field limit: Two-pulse control of IBr photofragmentation revisited

We demonstrate theoretically that laser-induced coherent quantum interference control of asymptotic states of dissociating molecules is possible, starting from a single vibrational eigenstate, after the interaction with two laser pulses—at a fixed time delay—both operating in the weak-field limit. Thus, phase dependence in the interaction with the second fixed-energy phase-modulated pulse persists after the pulse is over. This is illustrated for the nonadiabatic process: \( I + \text{Br} \rightarrow \text{IBr} \rightarrow I + \text{Br} \), where the relative yield of excited \( \text{Br}^* \) can be changed by pure phase modulation. Furthermore, a strong frequency dependence of the branching ratio is observed and related to the re-crossing dynamics of the avoided crossing in the above-mentioned process.

General information
State: Published
Organisations: Department of Chemistry
Authors: Tiwari, A. K. (Intern), Henriksen, N. E. (Intern)
Number of pages: 5
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Chemical Physics
Volume: 144
Issue number: 1
Article number: 014306
ISSN (Print): 0021-9606
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.13 SJR 1.073 SNIP 0.755
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.953 SNIP 0.767 CiteScore 1.98
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.386 SNIP 0.989 CiteScore 2.54
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.532 SNIP 1.17 CiteScore 2.95
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.787 SNIP 1.118 CiteScore 2.86
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.805 SNIP 1.207 CiteScore 3.07
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.73 SNIP 1.052
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.003 SNIP 1.104
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Phase Transitions in Layered Diguanidinium Hexachlorostannate(IV)

Five crystalline phases of diguanidinium hexachlorostannate(IV), \([\text{C(NH}_2(3)](2)\text{SnCl}_6\), have been identified and characterized by calorimetric and dielectric measurements, single crystal X-ray diffraction at atmospheric and high pressure, and synchrotron X-ray powder diffraction. The crystal structures of all phases are built of similar layers in which the tin hexachloride anions are connected to the guanidinium cations by N-H dot dot dot Cl hydrogen bonds, forming an interact primarily by Coulombic forces between the ions from ap. double H-bonded sheets. The layers, neutral as a whole, the opposing H-bonded sheets, and through the van der Waals contacts. From water solution the compound crystallizes at room temperature in phase III of space group C2/c. On heating, this phase transforms between 375 and 455 K to the high temperature phase I of space group P 1 over bar, either immediately or through the intermediate phase II of the same space group P 1 over bar. The temperature range of phase II enhances meaningfully at elevated pressure, which made possible the high-pressure crystallization of this phase and determination of its structure. Different transition paths can be realized when the crystal is cooled from phase I: the reverse transition occurs in the monoclinic phase III or in the monoclinic phase IV (space group C2/m), or in the phase V of space group PT. In all phases the layered structure of the crystal is preserved, while the arrangement of the layers is different. The transitions involve also transformations in the networks of N-H center dot dot dot Cl hydrogen bonds. The large volume (similar to 3%) and entropy (similar to R ln 3) change at the transition between phases II and III, and the giant pressure coefficient of -755 K GPa(-1), indicate a great potential of this material for applications in solid-state cooling systems.
Prediction of secondary metabolite encoding genes based on chemical structure analysis

General information

State: Published
Organisations: Department of Systems Biology, Department of Chemistry, Organic Chemistry, Eucaryotic Molecular Cell Biology
Authors: Petersen, T. I. (Intern), Nielsen, M. L. (Intern), Hoeck, C. (Intern), Frandsen, R. J. N. (Intern), Larsen, T. O. (Intern)
Number of pages: 1
Host publication information
Title of host publication: Book of abstracts from the 13th European Conference on Fungal Genetics
Article number: CS5T73
Main Research Area: Technical/natural sciences
Conference: 13th European Conference on Fungal Genetics, Paris, France, 03/04/2016 - 03/04/2016
Electronic versions:
Prediction of secondary metabolite encoding genes based on chemical structure analysis.pdf
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2016

Prediction of secondary metabolite encoding genes based on chemical structure analysis

General information
State: Published
Organisations: Department of Systems Biology, Natural Product Discovery, Department of Chemistry, Organic Chemistry, Eucaryotic Molecular Cell Biology, Metabolomics Platform, Ege University
Authors: Petersen, T. I. (Intern), Nielsen, M. L. (Intern), Hoeck, C. (Intern), Gezgin, Y. (Ekstern), Frandsen, R. J. N. (Intern), Nielsen, K. F. (Intern), Larsen, T. O. (Intern)
Number of pages: 1
Publication date: 2016
Conference: 9th Joint Meeting of AFERP, ASP, GA, JSP, PSE & SIF, Copenhagen, Denmark, 24/07/2016 - 24/07/2016
Main Research Area: Technical/natural sciences

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Journal: Planta Medica
Volume: 81
Issue number: S 01
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Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.97 SJR 0.654 SNIP 0.94
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.637 SNIP 0.991 CiteScore 2.1
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.762 SNIP 1.135 CiteScore 2.15
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.789 SNIP 1.246 CiteScore 2.37
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.75 SNIP 1.126 CiteScore 2.35
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.704 SNIP 1.144 CiteScore 2.23
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.771 SNIP 1.134
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.772 SNIP 1.096
BFI (2008): BFI-level 2
Probing spin-vibronic dynamics using femtosecond X-ray spectroscopy

Ultrafast pump-probe spectroscopy within the X-ray regime is now possible owing to the development of X-ray Free Electrons Lasers (X-FELs) and is opening new opportunities for the direct probing of femtosecond evolution of the nuclei, the electronic and spin degrees of freedom. In this contribution we use wavepacket dynamics of the photoexcited decay of a new Fe(ii) complex, [Fe(bmip)2]2+ (bmip = 2,6-bis(3-methyl-imidazole-1-ylidine)pyridine), to simulate the experimental observables associated with femtosecond Fe K-edge X-ray Absorption Near-Edge Structure (XANES) and X-ray emission (XES) spectroscopy. We show how the evolution of the nuclear wavepacket is translated into the spectroscopic signal and the sensitivity of these approaches for following excited state dynamics.

General information
State: Published
Organisations: Department of Chemistry, Newcastle University, Hungarian Academy of Sciences
Authors: Penfold, T. J. (Ekstern), Pápai, M. I. (Intern), Rozgonyi, T. (Ekstern), Møller, K. B. (Intern), Vankó, G. (Ekstern)
Number of pages: 16
Pages: 731-746
Publication date: 2016
Main Research Area: Technical/natural sciences

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Journal: Faraday Discussions
Volume: 194
ISSN (Print): 1359-6640
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.07 SJR 1.504 SNIP 0.925
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.51 SNIP 1.051 CiteScore 3.54
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.7 SNIP 1.278 CiteScore 3.79
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.618 SNIP 1.12 CiteScore 3.65
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Promoted V$_2$O$_5$/TiO$_2$ catalysts for selective catalytic reduction of NO with NH$_3$ at low temperatures

The influence of varying the V$_2$O$_5$ content (3–6 wt.%) was studied for the selective catalytic reduction (SCR) of nitrogen oxides by ammonia on heteropoly acid (HPA)- and tungsten oxide (WO$_3$)-promoted V$_2$O$_5$/TiO$_2$ catalysts. The SCR activity and alkali deactivation resistance of HPA-promoted V$_2$O$_5$/TiO$_2$ catalysts was found to be much higher than for WO$_3$-promoted catalysts. By increasing the vanadium content from 3 to 5 wt.% the catalysts displayed a two fold increase in activity at 225 °C and retained their initial activity after alkali doping at a molar K/V ratio of 0.181. Furthermore, the catalysts were characterized by N$_2$ physisorption, XRPD, NH$_3$-TPD, H$_2$-TPR, Raman, FTIR and EPR spectroscopy to investigate the properties of the catalysts. XRPD, Raman and FTIR showed that promotion by HPA instead of WO$_3$ causes the catalysts to possess a higher number of acid sites, both in fresh and alkali poisoned form, which might explain their higher potassium tolerance. Ex-situ EPR spectroscopy revealed that HPA-promoted catalysts have higher V$^{4+}$/V$^{5+}$ redox system, relative to WO$_3$.

General information
State: Published
Organisations: Department of Chemistry, Department of Chemical and Biochemical Engineering, Centre for Catalysis and Sustainable Chemistry, DTU Admission Course, CHEC Research Centre, Department of Chemistry
Pages: 282-290
Publication date: 2016
Main Research Area: Technical/natural sciences
SCR of NO with NH3, V2O5, Potassium poisoning, Heteropoly acids
Quinone-Enriched Gold Nanoparticles in Bioelectrochemistry and Charge Storage

We are aiming at the development of a general electrochemical platform suitable for multifarious investigations of biogenic materials. The new platform can be attained by grafting organic/metal hybrids with quinone functionality. In-house made and customized anthraquinone derivatives (with linking groups ranging from thiophenes to thiols) were chosen as model compounds for linking together bulk quantities of gold nanoparticles and providing desired functionality. Anthraquinone thiophene and thiol derivatives were synthetized via Sonogashira coupling-type reactions. The synthetic pathways for merging gold nanoparticles with resultant anthraquinones include one-pot microwave assisted synthesis or after-mixing of separately prepared gold nanoparticles with selected compounds. The quinone-enriched gold nanoparticles can be transferred onto different electrode surfaces, thus enabling facile manufacturing of functional electroactive films. Preliminary electrochemical investigations are indicative that quinone function is retained. The films can be utilized in broad energy related applications. Enzymes immobilized on the crafted new electrode materials can act as cathodes with “built-in” mediator for biofuel cells, or without any modification as anodes in putative and real charge storage devices. Moreover, the new anthraquinone derivatives offer interesting perspectives related with molecular electronics.

Reagent-Free Synthesis and Plasmonic Antioxidation of Unique Nanostructured Metal-Metal Oxide Core-Shell Microfibers

A photoresponsive inorganic microfiber with a plasmonic core–shell structure responds to visible light to achieve self-protection against oxidation in an open environment. The microfibers are synthesized via a newly developed reagent-free electrolytic method and have unique interfacial structures and high surface activity.
Reduction of hypervalent iodine by coordination to iron(III) and the crystal structures of PhiO and PhiO₂

The iodine L₃-edge X-ray Absorption Near Edge Structure (XANES) of organic and inorganic iodine compounds with formal iodine oxidation states ranging from -1 to +7 shows edge energies spanning from 4560.8 eV to 4572.5 eV. These were used to calibrate the oxidation state of iodine in a unique iron complex of iodosylbenzene (PhiO), [Fe(tpena)OIPh]^{2+} (tpena⁻ = N,N,N′-tris(2-pyridylmethyl)ethylenediamine-N’-acetate), which was found to be +1.6. Thus the iodine oxidation state is reduced by 1.4 compared with that in precursor uncoordinated PhiO. On the basis of a combination of X-ray diffraction and Extended X-ray Absorption Fine Structure (EXAFS) spectroscopy, we have determined the unknown crystal structure of PhiO, along with a new phase of iodylbenzene (β-PhiO₂) using the Rietveld method. Analogous 1-D chains of halogen bonded [O-IO-I] motifs are the dominant supramolecular interactions between PhiO and PhiO₂ monomers in each structure respectively and the polymeric structures rationalise the general insolubility of these oxygen atom transfer reagents. A double stack of phenyl units in PhiO is found between the layers of the halogen bonded OI chains. In the case of PhiO, C-Hπ interactions between adjacent phenyl groups result in the alternate phenyl groups lying in parallel planes. Supplementing the strong polymerizing halogen bonds, this supramolecular interaction must exacerbate the insolubility of PhiO. The pillared structure of the new rhombohedral β-PhiO₂ differs significantly from the known monoclinic lamellar phase, α-PhiO₂, described 36 years ago in which the chains form lamellar stacks [N. W. Alcock and J. F. Sawyer, J. Chem. Soc., Dalton Trans., 1980, 115-120].

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry, X-ray Crystallography, University of Southern Denmark
Authors: Wegeberg, C. (Ekstern), Frankær, C. G. (Intern), McKenzie, C. J. (Ekstern)
Release of Crude Oil from Silica and Calcium Carbonate Surfaces: On the Alternation of Surface and Molecular Forces by High- and Low-Salinity Aqueous Salt Solutions

Adsorption and desorption of a North Sea crude oil to silica and calcium carbonate surfaces were studied by a quartz crystal microbalance, while the bare surfaces and adsorbed oil layers were characterized by atomic force microscopy and contact angle measurements. Water contact angles were measured on the bare surfaces, surfaces with an adsorbed oil layer, and surfaces after being exposed to aqueous salt solutions. This showed that the silica surface became more hydrophobic after oil adsorption, while the wettability of the calcium carbonate surface was not significantly changed by adsorption of an oil layer. A surface energy component analysis based on the acid base theory showed that oil adsorption on the surfaces depends upon apolar, acidic, and basic oil components of the crude oil and that the adsorbed oil components differ for adsorption to silica and calcium carbonate. Desorption of the crude oil was investigated by exposing the surfaces with an adsorbed oil layer to a series of NaCl and CaCl₂ solutions of decreasing salt concentrations. Here, it was found that the oil release from silica was achieved only by injections of low-salinity solutions, and it is suggested that this observation is due to an expansion of the electrical double layer. The oil release from calcium carbonate was achieved by injection of both high- and low-salinity solutions of NaCl but not injection of a high-salinity solution of CaCl₂. These observation are attributed to dissolution of calcium carbonate or reduction in ion bridging in the presence of high-salinity NaCl, while the low-salinity effect again was attributed to an expansion of the electrical double layer.
Reversible devitrification in amorphous $\text{As}_2\text{Se}_3$ under pressure

In pressure-induced reversible structural transitions, the term "reversible" refers to the recovery of the virgin structure in a material upon complete decompression. Pressure-induced amorphous-to-crystalline transitions have been claimed to be reversible, but evidence that amorphous material recovers its virgin amorphous structure upon complete depressurization has been lacking. In amorphous $\text{As}_2\text{Se}_3$ ($\alpha$-$\text{As}_2\text{Se}_3$) chalcogenide, however, we report a novel reversible amorphous-to-crystalline transition that provides compelling experimental evidence that upon complete decompression, the recovered amorphous phase is structurally the same as that of the virgin (as-cast) amorphous phase. Combining the experimental results with ab initio molecular dynamics simulations, we elucidate that the amorphization is mediated by a surplus of total free energy in the high-pressure face-centered cubic phase as compared to the virgin amorphous phase and that the structural recovery to the virgin amorphous phase is a consequence of an enhancement in covalent bonding character over interlayer forces upon complete decompression. Furthermore, we observed a two-dimensional to three-dimensional network transition under compression and its reversibility upon decompression.

General information

State: Published
Organisations: Department of Chemistry, X-ray Crystallography, Zhejiang University, Chinese Academy of Sciences, Deutsches Elektronen-Synchrotron, Universite de Rennes 1, University of Cambridge
Authors: Ahmad, A. S. (Ekstern), Lou, H. B. (Ekstern), Lin, C. L. (Ekstern), Li, A. G. (Ekstern), Yang, K. (Ekstern), Glazyrin, K. (Ekstern), Liermann, H. P. (Ekstern), Franz, H. (Ekstern), Ståhl, K. (Intern), Cui, S. (Ekstern), Bureau, B. (Ekstern), Zhang, D. (Ekstern), Wang, X. (Ekstern), Cao, Q. (Ekstern), Greer, A. L. (Ekstern), Jiang, J. (Ekstern)
Number of pages: 7
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: Physical Review B
Sandwich-like functionalized free-standing and flexible graphene papers for supercapacitors

The development of flexible and free-standing electrodes is a key step for fabrication of flexible and compact electronic and energy devices which is of significant interests in portable electronics. This is increasingly demanded by modern electronics, portable medical products, and compact energy devices. Hybrid electrodes with functional nanocrystals anchored on carbon substrates are under intense research for a broad spectrum of applications in sensing, energy conversion and storage, and catalysis. Among carbon materials, graphene, consisting of a single-layer of sp²-hybridized carbon atoms, has emerged as a new class of supporting scaffolds for nanocrystals because of a unique collection of structural and electronic properties such as large surface areas, chemical inertness, and superior electrical conductivity. As a two-dimensional (2D) transition metal dichalcogenide (TMDC), tin disulfide (SnS₂) is a promising material for multiple applications in supercapacitors, lithium ion batteries and photocatalysis due to its excellent optical and electrical properties. In this poster, we present a facile approach to the preparation of sandwich-like paper electrodes with Au nanoparticle-decorated reduced graphene oxide paper (rGOPAuNPs) as substrates and 2D SnS₂ nanoflake-anchored reduced graphene oxide (SnS₂@rGO) nanosheets as high-performance supercapacitive material. The 2D self-assemblies of Au nanoparticles (AuNPs) on the surface of graphene papers can enhance electrode conductivity and facilitate electron transfer between rGOP and SnS₂@rGO, as well as serve as a strength reinforcing component by forming stable Au-S bonds. The proposed paper electrodes show the combined advantages contributed from both graphene paper substrates and self-assembled AuNPs layers as well as could improve conductivity of 2D SnS₂ nanoflakes. Our results show the promise that this approach could evolve to be a universal strategy for practical fabrication of multifunctional flexible portable paper electrodes for energy storage and sensing devices.

General information
State: Published
Organisations: Department of Chemistry, NanoChemistry, Organic Chemistry
Authors: Cao, X. (Intern), Duus, J. Ø. (Intern), Chi, Q. (Intern)
Number of pages: 1
Publication date: 2016
Main Research Area: Technical/natural sciences
Links:
http://www.sustain.dtu.dk/

Bibliographical note
Sustain Abstract M-13
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2016

Selective H₂S removal from bio-methane gas by ionic liquid technology

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry
Authors: Schill, L. (Intern), Fehrmann, R. (Intern), Riisager, A. (Intern)
Number of pages: 1
Publication date: 2016
Main Research Area: Technical/natural sciences
Links:
http://www.sustain.dtu.dk/

Bibliographical note
Sustain Abstract E-18
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2016

Selective Reversible Absorption of the Industrial Off-Gas Components CO₂ and NOₓ by Ionic Liquids

Ionic liquids are promising new materials for climate and pollution control by selective absorption of CO₂ and NOₓ in industrial off-gases. In addition practical cleaning of industrial off gases seems to be attractive by use of ionic liquids distributed on the surface of porous, high surface area carriers in the form of so-called Supported Ionic Liquid Phase (SIILP) materials. The potential of selected ionic liquids for absorption of CO₂ and NOₓ are demonstrated and the possible interference of other gases influencing the stability and absorption capacity of the ionic liquids are investigated as well.

General information
State: Published
Selective Reversible Absorption of the Industrial Off-Gas Components CO₂ and NOₓ by Ionic Liquids

Ionic liquids are promising new materials for climate and pollution control by selective absorption of CO₂ and NOₓ in industrial off-gases. In addition, practical cleaning of industrial off gases seems to be attractive by use of ionic liquids distributed on the surface of porous, high surface area carriers in the form of so-called Supported Ionic Liquid Phase (SILP) materials. The potential of selected ionic liquids for absorption of CO₂ and NOₓ will be demonstrated and the possible mechanism of absorption will be described on the molecular level. Our vision of application of these ionic liquids in the form of SILP filters to flue gas cleaning in power plants, waste incineration plants, cement and glass factories as well as unborad ships will be addressed.

General information
State: Published
Shape-selective Valorization of Biomass-derived Glycolaldehyde using Tin-containing Zeolites

A highly selective self-condensation of glycolaldehyde to different C4 molecules has been achieved using Lewis acidic stannosilicate catalysts in water at moderate temperatures (40–100 °C). The medium-sized zeolite pores (10-membered ring framework) in Sn-MFI facilitate the formation of tetrose sugars while hindering consecutive aldol reactions leading to hexose sugars. High yields of tetrose sugars (74 %) with minor amounts of vinyl glycolic acid (VGA), an α-hydroxyacid, are obtained using Sn-MFI with selectivities towards C4 products reaching 97 %. Tin catalysts having large pores or no pore structure (Sn-Beta, Sn-MCM-41, Sn-SBA-15, tin chloride) led to lower selectivities for C4 sugars due to formation of hexose sugars. In the case of Sn-Beta, VGA is the main product (30 %), illustrating differences in selectivity of the Sn sites in the different frameworks. Under optimized conditions, GA can undergo further conversion, leading to yields of up to 44 % of VGA using Sn-MFI in water. The use of Sn-MFI offers multiple possibilities for valorization of biomass-derived GA in water under mild conditions selectively producing C4 molecules.
Aldol condensation, Biomass conversion, Tetrose sugars, Tin, Zeolites

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Source: FindIt
Source-ID: 2342289564
Publication: Research - peer-review › Journal article – Annual report year: 2016

Side Effect of Good's Buffers on Optical Properties of Gold Nanoparticle Solutions
In search of fluorescent nanoclusters (NCs) for bioimaging, several methods of synthesis have been attempted. Particularly, formation of gold NCs (AuNCs) during synthesis of gold nanoparticles (AuNPs) using Good's buffers was reported based on the optical properties of the reactions mixtures. Here we chose the Good's buffers 2-(N-morpholino)ethanesulfonic acid (MES), 3-(N-morpholino)propanesulfonic acid (MOPS) and 4-(N-morpholino)butanesulfonic acid (MOBS) as [AuCl4]- reducing agents. Resulting AuNP solutions were subjected to electrochemical investigations along with UV-vis and fluorescence spectroscopy. Distinct absorption features at ca. 290 and 360 nm and fluorescence emission in the 408-484 nm range are observed in filtered AuNP-free solutions. Electrochemical oxidation of these buffers generates similar optical properties, suggesting that the degradation products of the buffers contribute to the optical properties of AuNP solutions. This work indicates deeper evaluation of fluorescence signals based on metal NPs or NCs is needed.

General information
State: Published
Organisations: Department of Chemistry, NanoChemistry, Organic Chemistry, Metalloprotein Chemistry and Engineering, Technical University of Denmark, East China University of Science and Technology
Authors: Engelbrekt, C. (Intern), Wagner, M. (Intern), Undall-Behrend Christiansen, M. (Forskerdatabase), Christensen, H. E. M. (Intern), Qian, X. (Ekstern), Ulstrup, J. (Intern), Zhao, C. (Ekstern), Zhang, J. (Intern)
Number of pages: 7
Pages: 1212-1218
Publication date: 2016
Main Research Area: Technical/natural sciences

Publication information
Journal: ChemElectroChem
Volume: 3
Issue number: 8
ISSN (Print): 2196-0216
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BFI (2018): BFI-level 1
Gold nanoparticles, Gold nanoclusters, Good’s buffers, Cyclic voltammetry, Fluorescence

DOIs:
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Source: FindIt
Source-ID: 2305873134
Publication: Research - peer-review › Journal article – Annual report year: 2016

Single center reactivity of Cu(II) sites in copper substituted CHA zeolite followed by in-situ electron paramagnetic resonance spectroscopy

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry, Haldor Topsoe AS, Technical University of Denmark
Authors: Mossin, S. (Intern), Isaksen, O. (Ekstern), Godiksen, A. (Intern), Rasmussen, S. B. (Ekstern), Vennestøm, P. N. R. (Ekstern)
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Relations
Activities:
Single center reactivity of Cu(II) sites in copper substituted CHA zeolite followed by in-situ electron paramagnetic resonance spectroscopy
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2017

Single-Nanoparticle Resolved Biomimetic Long-Range Electron Transfer and Electrocatalysis of Mixed-Valence Nanoparticles

Long-range electron transfer (LRET) is a core elementary step in a wealth of processes central to chemistry and biology, including photosynthesis, respiration, and catalysis. In nature, biological catalysis is performed by enzymes. However, enzymes are structurally fragile and have limited stability in vitro. Development of robust biomimetic nanostructures is therefore highly desirable. Here, with Prussian blue nanoparticles (PBNPs) as an example we have demonstrated the preparation of highly stable and water-soluble mixed-valence nanoparticles under mild conditions. We have mapped their enzyme-mimicking catalytic properties and controlled LRET to single-nanoparticle resolution. PBNPs show high substrate binding affinity and tunable electrocatalytic efficiency toward hydrogen peroxide reduction, resembling the patterns for similar size redox metalloenzymes. We have further disclosed a correlation between electrocatalytic efficiency and distance-dependent interfacial ET kinetics. Given their high stability and low cost, such enzyme-mimicking nanoparticles could offer new perspectives in the fields of catalysis, sensors, and electrochemical energy conversion.

General information
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Organisations: NanoChemistry, Department of Chemistry, Organic Chemistry
Authors: Zhu, N. (Intern), Hao, X. (Intern), Ulstrup, J. (Intern), Chi, Q. (Intern)
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Small-molecule kinase inhibitors: an analysis of FDA-approved drugs

Small-molecule kinase inhibitors (SMKIs), 28 of which are approved by the US Food and Drug Administration (FDA), have been actively pursued as promising targeted therapeutics. Here, we assess the key structural and physicochemical properties, target selectivity and mechanism of function, and therapeutic indications of these approved inhibitors. Our analysis showed that >30% of approved SMKIs have a molecule weight (MW) exceeding 500 and all have a total ring count of between three and five. The assumption that type II inhibitors tend to be more selective than type I inhibitors has been proved to be unreliable. Although previous SMKI research was concentrated on tyrosine kinase inhibitors for cancer treatment, recent progress indicates diversification of SMKI research in terms of new targets, mechanistic types, and therapeutic indications.
Solution behaviour of Human Serum Albumin and GLP-1 variants

The formation of macromolecular complexes and the solution behaviour of proteins are results of protein-protein interactions (PPI) and the nature of the solution components. PPI's can be divided into two broad categories of attractive and repulsive forces. From a formulation perspective, proper interaction is critical for the long term stability of a pharmaceutical. Protein complex formation is important for extended half-life in vivo and is essential to cellular communication such as the induction of the insulin response.

This thesis focuses on human serum albumin (HSA) as a central player and the ability of small-angle X-ray scattering (SAXS) to study proteins under diverse solution conditions. HSA is utilized in many ways in the pharmaceutical industry such as the formulations of other proteins and in particular for half-life extension of peptides, where the long half-life of up
to 21 days of HSA is deployed. The thesis is divided into four parts: 1) Self-interaction of HSA in pharmaceutical relevant systems; 2) The liraglutide oligomer and interaction with HSA; 3) Conjugation of GLP-1 to HSA and last but not least 4) A benchmark study of the implementation of SAXS in RosettaDock.

HSA is used as a stabilizer in formulation where it is known to decrease adsorption to the air/liquid and liquid/container interfaces, thereby reducing the aggregation propensity of the target protein. However, with high concentration liquid formulations coming into focus limited information is available on the behaviour of HSA in these crowded environments. We have applied SAXS in order to shed light on the self-interaction of HSA in pharmaceutical relevant buffer systems on protein concentrations up to 150 mg/ml. HSA stabilized by octanoate is observed to interact by purely repulsive forces in the investigated concentration ranges while defatted HSA show attractive forces at low protein concentration. The toxicity corresponding to isotonicity, is observed to coincide with the maximum screening observed in all systems while this is not observed as a function of ionic strength, making toxicity an important parameter for protein interaction in the investigated systems. Trehalose is seen to provide a screening effect of added NaCl leading us to think that trehalose somehow determines the range of interaction of the proteins in solution. Finally it is proposed that the stabilizing effect of HSA could be mediated by a repulsive network of HSA molecules screening the interaction of other proteins, hereby decreasing the aggregation propensity.

Glucagon-like peptide 1 (GLP-1) is an incretin hormone used in the treatment of diabetes mellitus type 2. Due to its very limited half-life of approximately 3 minutes, Novo Nordisk A/S developed an acylated analogue, liraglutide, which due to multimerization and probable interaction with HSA in-vivo, makes it applicable for once daily administration. The oligomerization and the interaction with HSA were investigated by SAXS and static light scattering (SLS). The oligomeric state of liraglutide was approximately heptameric but due to uncertainties, the experimental studies were complimented by a series of molecular dynamic (MD) simulations. The results from MD where compared to the experimental SAXS data and the combined effort show that the liraglutide heptamer was the most probable multimer. The studies of liraglutide with HSA both in a defatted form and a stabilized form, were capable of confirming the presence of a hetero complex though at very low concentration. This could be a result of very transient interaction or the consequence of non-optimal buffer conditions.

Another approach to half-life extension is conjugation of molecules to HSA. In this part of the thesis, novel GLP-1-albumin conjugates developed by Albumedix A/S where examined by a combined approach of pharmacokinetic studies and solution structure determination with SAXS. GLP-1 was conjugated to Cys34 of recombinant HSA (rHSA) and two rHSA variants with lower (NB) and higher binding (HB) affinity to the neonatal Fc receptor (FcRn). Binding kinetics showed that the conjugation had limited effect on the binding properties of the conjugates to FcRn compared to the respective rHSA variants. Increased in-vivo half-life of the conjugates was observed in NMRI WT mice compared to GLP-1, with the HB-variant displaying ~300 times longer half-life, while the potency of GLP-1-albumin was decreased by 3-4 orders of magnitude compared to GLP-1. The solution structure of the rHSA variants and the conjugates indicate a flexible nature of the conjugate, with the GLP-1 pointing away from the surface of rHSA. The low resolution structure from SAXS combined with high resolution structural information from X-ray crystallography, explains the pharmacokinetics results, as limited interference is seen between FcRn and the conjugate, while albumin steric hindrance explains the decreased potency of the conjugates.

Structure determination of macromolecular complexes can be challenging by traditional approaches such as X-ray crystallography and NMR. An alternative approach is the use of experimental knowledge in combination with in-silico modelling to gain knowledge about macromolecular complexes. The final part of the thesis regards the benchmarking of the protein docking tool, RosettaDock, in combination with SAXS. The RosettaDock protocol is a two-step process involving a low resolution rigid body protocol, set up to imitate the initial protein-protein encounter, followed by a high resolution protocol where the position of the proteins and amino acid side chains are optimized. We applied SAXS as constrain (SAXSconstrain) after the low resolution step to filter out complexes with overall shapes which would not match the SAXS data. Since it is a rigid body approach larger conformational changes in any part of the complex provides a limit to the method either from interface non-complementarity or a resulting shape which deviates from the SAXS data. 38 structures from Benchmark 4.0 of different difficulty levels were investigated using this approach. In general our result indicate that implementation of SAXSconstrain reduces the sampling space and increases the probability of finding a near-native structure. In a wider perspective, the strength of RosettaDockSAXS lies in the combination of low-resolution structural information from SAXS experiments and the protein-protein interaction energies obtained from RosettaDock which provides means to gain insight to higher resolution information about the interface between two protein partners. This allows for the prediction of unknown three-dimensional atomic structures of protein-protein complexes.

General information
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Authors: Sønderby, P. (Intern), Harris, P. (Intern), Peters, G. H. (Intern)
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Solving a 3D structural puzzle

Nuclear magnetic resonance (NMR) spectroscopy is a versatile tool in analytical chemistry, highly suitable for structural elucidation of organic molecules – as well as multiple other areas of research. The subjects covered within this thesis all concern methods which allow a shift from covalent to spatial structural information using NMR spectroscopy. Experimental distances from nuclear Overhauser effect (NOE) correlations, and dihedral angles from 3JHH-coupling constants, were used to obtain 3D structural information for several natural and synthetic compounds. The stereochemistry of novel natural compounds was determined, including that of a bicyclic non-ribosomal peptide (a novel structural motif), a steroid and several polyketides.

Structural insights were gained for potential anti-cancer agents; the azumamides, including synthetic analogues. Differences in the conformational space of solution state compounds were identified experimentally between structural analogues, and compared to the in vitro potency of the compounds. The structures of two peptides that exhibited a high degree of molecular recognition were investigated, resulting in the elucidation of a possible mode of interaction. Also a major assumption in the calculation of distances from NOEs, the assumption of equal rotational correlation times between proton pairs, was investigated for molecules in organic solvents.

Two spin-state selective (S3) HMBC experiments were developed for measurements of homonuclear and heteronuclear long-range coupling constants, respectively. The new NMR experiments were based on two existing experiments, the multiplicity edited HMBC and the HAT HMBC, which were combined to obtain S3 editing of long-range homonuclear coupling constants. The output of the first S3 HMBC experiment was HMBC type spectra with nJCH correlated crosspeaks, from which n+1JHH-coupling constants were sign-selectively determined with high accuracy. Very small coupling constants, including previously unreported coupling constants from strychnine, were extracted, with all experimental values correlating very well to theoretical coupling constants from DFT calculation. A pulse segment was developed to change the polarization of the CH-H pairs in the homonuclear S3 HMBC, to gain S3 edited nJCH-coupling constants in the cross-peaks. While only determining coupling constants to methine carbons, the extracted experimental coupling constants correlated very well to theoretical coupling constants, thus extending the S3 HMBC methodology to include both n+1JHH- and nJCH-coupling constants. Residual dipolar couplings (RDCs) are a relatively late addition to the NMR community, where alignment media are used to obtain anisotropic samples, which allows for RDCs to be extracted. The number of internuclear vectors for the correlation of RDCs to 3D structures is often limited for small molecules. Homonuclear RDCs were extracted by use of the homonuclear S3 HMBC that correlated well to alignment tensors from 1DCH-coupling constants, thus increasing the number of inter-nuclear vectors. The topic of enantiodiscrimination by RDC measurements of rigid organic molecules was also investigated, and new alignment media were developed to allow slight discrimination of enantiomers by stretched polymers. Finally a new method of back-calculation of RDCs from 3D structures was developed and tested, which copes better with multiple conformers than the commonly used SVD methodology. The approach thus resulted in good conformer populations for several small molecules, including multiple cinchona alkaloids.

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Solving a 3D structural puzzle

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Specific electrical conductivity in molten potassium dihydrogen phosphate KH$_2$PO$_4$ - An electrolyte for water electrolysis at ~300°C

The conductivity of pure molten KH$_2$PO$_4$ salt and four mixtures with more or less water (KH$_2$PO$_4$-H$_2$O and KH$_2$PO$_4$-KPO$_3$ systems, respectively) were measured at temperatures of 240-320°C and under their own water vapor pressures. Molten KH$_2$PO$_4$ has been proven to be a promising electrolyte for an elevated temperature pressurized water electrolyzer demonstrating high conductivity of ~0.30 S cm$^{-1}$ at 300°C. The conductivity data are given as polynomial functions of temperature and composition. The melting point of the pure salt under its own water vapor pressure was determined to be ~272°C.

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Organisations: Department of Energy Conversion and Storage, Proton conductors, Department of Chemistry
Authors: Nikiforov, A. V. (Intern), Berg, R. W. (Intern), Petrushina, I. (Intern), Bjerrum, N. J. (Intern)
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Scopus rating (2016): CiteScore 7.78 SJR 3.058 SNIP 2.573
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 2.912 SNIP 2.61 CiteScore 6.4
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 3.254 SNIP 3.28 CiteScore 6.93
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 3.164 SNIP 3.377 CiteScore 6.59
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.854 SNIP 3.108 CiteScore 5.69
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.473 SNIP 2.84 CiteScore 5.5
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.516 SNIP 2.25
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.003 SNIP 1.781
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 0.974 SNIP 1.215
Specific Electrostatic Molecular Recognition in Water

The identification of pairs of small peptides that recognize each other in water exclusively through electrostatic interactions is reported. The target peptide and a structure-biased combinatorial ligand library consisting of ≈78,125 compounds were synthesized on different sized beads. Peptide–peptide interactions could conveniently be observed by clustering of the small, fluorescently labeled target beads on the surface of larger ligand-containing beads. Sequences of isolated hits were determined by MS/MS. The interactions of the complex showing the highest affinity were investigated by a novel single-bead binding assay and by 2D NMR spectroscopy. Molecular dynamics (MD) studies revealed a putative mode of interaction for this unusual electrostatic binding event. High binding specificity occurred through a combination of topological matching and electrostatic and hydrogen-bond complementarities. From MD simulations binding also seemed to involve three tightly bound water molecules in the interface between the binding partners. Binding constants in the submicromolar range, useful for biomolecular adhesion and in nanostructure design, were measured.

General information

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Organisations: Department of Chemistry, Organic Chemistry, University of Copenhagen
Authors: Li, M. (Ekstern), Hoeck, C. (Intern), Schoffelen, S. (Ekstern), Gottfredsen, C. H. (Intern), Meldal, M. (Ekstern)
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Scopus rating (2016): CiteScore 5.03 SJR 2.247 SNIP 1.046
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 2.416 SNIP 1.184 CiteScore 4.99
Spectroscopic approaches to resolving ambiguities of hyper-polarized NMR signals from different reaction cascades

The influx of exogenous substrates into cellular reaction cascades on the seconds time scale is directly observable by NMR spectroscopy when using nuclear spin polarization enhancement. Conventional NMR assignment spectra for the identification of reaction intermediates are not applicable in these experiments due to the non-equilibrium nature of the nuclear spin polarization enhancement. We show that ambiguities in the intracellular identification of transient reaction intermediates can be resolved by experimental schemes using site-specific isotope labelling, optimised referencing and response to external perturbations.
S$^3$ HMBC: Spin-State-Selective HMBC for accurate measurement of homonuclear coupling constants. Application to strychnine yielding thirteen hitherto unreported J$_{HH}$

A novel method, Spin-State-Selective (S$^3$) HMBC, for accurate measurement of homonuclear coupling constants is introduced. As characteristic for S$^3$ techniques, S$^3$ HMBC yields independent subspectra corresponding to particular passive spin states and thus allows determination of coupling constants between detected spins and homonuclear coupling partners along with relative signs. In the presented S$^3$ HMBC experiment, spin-state selection occurs via large one-bond coupling constants ensuring high editing accuracy and unequivocal sign determination of the homonuclear long-range relative to the associated one-bond coupling constant. The sensitivity of the new experiment is comparable to that of regular edited HMBC and the accuracy of the J/RDC measurement is as usual for E.COSY and S$^3$-type experiments independent of the size of the homonuclear coupling constant of interest. The merits of the method are demonstrated by an application to strychnine where thirteen J$_{HH}$ coupling constants not previously reported could be measured.
Stabilization of Tryptophan Hydroxylase 2 by L-Phenylalanine Induced Dimerization

Tryptophan hydroxylase 2 (TPH2) catalyses the initial and rate-limiting step in the biosynthesis of serotonin, which is associated with a variety of disorders such as depression, obsessive compulsive disorder, and schizophrenia. Full length TPH2 is poorly characterized due to low purification quantities caused by its inherent instability. Three truncated variants of human TPH2 (rchTPH2; regulatory and catalytic domain, NΔ47-rchTPH2; truncation of 47 residues in the N-terminus of rchTPH2, and chTPH2; catalytic domain) were expressed, purified, and examined for changes in transition temperature, inactivation rate, and oligomeric state. chTPH2 displayed 14- and 11-fold higher half-lives compared to rchTPH2 and NΔ47-rchTPH2, respectively. Differential scanning calorimetry experiments demonstrated that this is caused by premature unfolding of the less stable regulatory domain. By differential scanning fluorimetry, the unfolding transitions of rchTPH2 and NΔ47-rchTPH2 are found to shift from polyphasic to apparent two-state by the addition of L-Trp or L-Phe. Analytical gel filtration revealed that rchTPH2 and NΔ47-rchTPH2 reside in a monomer-dimer equilibrium which is significantly shifted towards dimer in the presence of L-Phe. The dimerizing effect induced by L-Phe is accompanied by a stabilizing effect, which resulted in a 3-fold increase in half-lives of rchTPH2 and NΔ47-rchTPH2. Addition of L-Phe to the purification buffer significantly increases the purification yields, which will facilitate characterization of hTPH2.
Strain development during the phase transition of $\text{La(Fe,Mn,Si)}_{13} H_2$

We use powder X-ray diffraction to evaluate the temperature dependence of the crystalline properties during the magnetic phase transition of $\text{La(Fe,Mn,Si)}_{13} H_2$ as a function of the Fe/Mn/Si ratio. Both the paramagnetic and ferromagnetic phases were observed as peak overlaps in the patterns around the Curie temperature ($T_C$) occurring continuously in a temperature range of about 5 K around $T_C$. Using the Williamson-Hall method, we evaluate the strain developing in the crystallites during the transition and find that it is associated with the growth of the paramagnetic phase as the transition occurs. Based on our measurements and microstructure analyses, we propose that cracking during the phase transition is due to or aggravated by the small content of a La-rich phase.

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Organisations: Electrofunctional materials, Department of Energy Conversion and Storage, Atomic scale modelling and materials, Department of Chemistry, X-ray Crystallography
Authors: Neves Bez, H. (Intern), Nielsen, K. K. (Intern), Smith, A. (Intern), Norby, P. (Intern), Ståhl, K. (Intern), Bahl, C. R. H. (Intern)
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Web of Science (2016): Indexed yes
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Scopus rating (2015): SJR 1.085 SNIP 0.983 CiteScore 2.47
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Strategies for improving the solubility and metabolic stability of griseofulvin analogues

We report two types of modifications to the natural product griseofulvin as strategies to improve solubility and metabolic stability: the conversion of aryl methyl ethers into aryl difluoromethyl ethers at metabolic hotspots and the conversion of the C-ring ketone into polar oximes. The syntheses of the analogues are described together with their solubility, metabolic half-life in vitro and antiproliferative effect in two cancer cell lines. We conclude that on balance, the formation of polar oximes is the most promising strategy for improving the properties of the analogues.
Griseofulvin analogues, Anticancer, Synthesis, Antifungal, Metabolic stability

Structure and dynamics of water and lipid molecules in charged anionic DMPG lipid bilayer membranes

Molecular dynamics simulations have been used to investigate the influence of the valency of counter-ions on the structure of freestanding bilayer membranes of the anionic 1,2-dimyristoyl-sn-glycero-3-phosphoglycerol (DMPG) lipid at 310 K and 1 atm. At this temperature, the membrane is in the fluid phase with a monovalent counter-ion and in the gel phase with a divalent counter-ion. The diffusion constant of water as a function of its depth in the membrane has been determined from mean-square-displacement calculations. Also, calculated incoherent quasielastic neutron scattering functions have been compared to experimental results and used to determine an average diffusion constant for all water molecules in the system. On extrapolating the diffusion constants inferred experimentally to a temperature of 310 K, reasonable agreement with the simulations is obtained. However, the experiments do not have the sensitivity to confirm the diffusion of a small component of water bound to the lipids as found in the simulations. In addition, the orientation of the dipole moment of the water molecules has been determined as a function of their depth in the membrane. Previous indirect estimates of the electrostatic potential within phospholipid membranes imply an enormous electric field of $10^8-10^9$ V m$^{-1}$, which is likely to have great significance in controlling the conformation of translocating membrane proteins and in the transfer of ions and molecules across the membrane. We have calculated the membrane potential for DMPG bilayers and found $\sim 1$ V ($\sim 2 \cdot 10^8$ V m$^{-1}$) when in the fluid phase with a monovalent counter-ion and $\sim 1.4$ V ($\sim 2.8 \cdot 10^8$ V m$^{-1}$) when in the gel phase with a divalent counter-ion. The number of water molecules for a fully hydrated DMPG membrane has been estimated to be 9.7 molecules per lipid in the gel phase and 17.5 molecules in the fluid phase, considerably smaller than inferred experimentally for 1,2-dimyristoyl-sn-glycero-3-phosphorylcholine (DMPC) membranes but comparable to the number inferred for 1,2-dilauroyl-sn-glycero-3-phosphoethanolamine (DLPE) membranes. Some of the properties of the DMPG membrane are compared with those of the neutral zwitterionic DMPC bilayer membrane at 303 K and 1 atm, which is the same reduced temperature with respect to the gel-to-fluid transition temperature as 310 K is for the DMPG bilayer membrane.
Structure of branching enzyme- and amylomaltase modified starch produced from well-defined amylose to amylopectin substrates

Thermostable branching enzyme (BE, EC 2.4.1.18) from Rhodothermus obamensis in combination with amylomaltase (AM, EC 2.4.1.25) from Thermus thermophilus was used to modify starch structure exploring potentials to extensively increase the number of branch points in starch. Amylose is an important constituent in starch and the effect of amylose on enzyme catalysis was investigated using amylose-only barley starch (AO) and waxy maize starch (WX) in well-defined ratios. All products were analysed for amylopectin chain length distribution, α-1,6 glucosidic linkages content, molar mass distribution and digestibility by using rat intestinal α-glucosidases. For each enzyme treatment series, increased AO content resulted in a higher rate of α-1,6 glucosidic linkage formation but as an effect of the very low initial branching of the AO, the final content of α-1,6 glucosidic linkages was slightly lower as compared to the high amylopectin substrates. However, an increase specifically in short chains was produced at high AO levels. The molar mass distribution for the
enzyme treated samples was lower as compared with substrate WX and AO, indicating the presence of hydrolytic activity as well as cyclisation of the substrate. For all samples, increased amylose substrate showed decreased α- and β-amylolysis. Surprisingly, hydrolysis with rat intestinal α-glucosidases was higher with increasing α-1,6 glucosidic linkage content and decreasing Mw, indicating that steric hindrance towards the α-glucosidases was directed by the molar mass rather than the branching density of the glucan per se. Our data demonstrate that a higher amylose content in the substrate starch efficiently produces α-1,6 glucosidic linkages and that the present of amylose generates a higher Mw and more resistant product than amylpectin. The combination of BE → AM → BE provided somewhat more resistant α-glucan products as compared to BE alone.

**General information**

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BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 5.15 SJR 1.404 SNIP 1.745
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.46 SNIP 1.842 CiteScore 4.86
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.584 SNIP 1.969 CiteScore 4.69
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.346 SNIP 1.967 CiteScore 4.39
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.409 SNIP 2.045 CiteScore 3.93
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.287 SNIP 1.991 CiteScore 4.08
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.372 SNIP 1.808
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.43 SNIP 1.718
BFI (2008): BFI-level 1
Study of the Polarization Behavior of Ce$_{0.9}$Gd$_{0.1}$O$_{2-\delta}$ Single Crystals below 350°C to Room Temperature

Single crystalline ceria samples with the composition Ce$_{0.9}$Gd$_{0.1}$O$_{2-\delta}$ were pre-polarized with ±5 V for up to 300 s using a Pt coated AFM tip as working electrode. The direct contact zone had a diameter of <50 nm. Subsequently, the effect of the polarization on the surface potential of the samples was investigated by mapping the introduced defect gradient and its decay with time using Kelvin probe force microscopy. The generated surface potential gradients were found to have a diameter of up to 1 μm, which is explained by the local ionization of defect associates by the applied high electric field. Measurements were performed at room temperature and 50°C. The polarization behavior of the Ce$_{0.9}$Gd$_{0.1}$O$_{2-\delta}$ single crystals was compared to cyclovoltammetry and polarization-relaxation experiments at T ≤ 350°C and in dry air or nitrogen which were performed using a specially suited AFM (Controlled Atmosphere High Temperature Scanning Probe Microscope CAHT-SPM by Semilab).

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Scopus rating (2016): CiteScore 2.97 SJR 1.134 SNIP 0.867
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BFI (2015): BFI-level 1
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Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.147 SNIP 1.206 CiteScore 3.36
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.151 SNIP 1.299 CiteScore 2.92
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.329 SNIP 1.296 CiteScore 2.61
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.33 SNIP 1.345 CiteScore 2.74
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.417 SNIP 1.312
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.45 SNIP 1.267
Web of Science (2009): Indexed yes
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Scopus rating (2007): SJR 1.58 SNIP 1.325
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.611 SNIP 1.54
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.519 SNIP 1.484
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.719 SNIP 1.706
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.962 SNIP 1.679
Web of Science (2003): Indexed yes
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Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 1.651 SNIP 1.738
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Study_of_the_Polarization_Behavior_of_Ce0.9Gd0.1O2_Single_Crystals_below_350_C_to_Room_Temperature_postprint.pdf
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Publication: Research - peer-review › Journal article – Annual report year: 2016
1H-13C NMR-based profiling of biotechnological starch utilization

Starch is used in food-and non-food applications as a renewable and degradable source of carbon and energy. Insight into the chemical detail of starch degradation remains challenging as the starch constituents amylose and amyllopectin are homopolymers. We show that considerable molecular detail of starch fragmentation can be obtained from multivariate analysis of spectral features in optimized 1H-13C NMR spectroscopy of starch fragments to identify relevant features that distinguish processes in starch utilization. As a case study, we compare the profiles of starch fragments in commercial beer samples. Spectroscopic profiles of homooligomeric starch fragments can be excellent indicators of process conditions. In addition, differences in the structure and composition of starch fragments have predictive value for downstream process output such as ethanol production from starch. Thus, high-resolution 1H-13C NMR spectroscopic profiles of homooligomeric fragment mixtures in conjunction with chemometric methods provide a useful addition to the analytical chemistry toolbox of biotechnological starch utilization.

General information
State: Published
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Scopus rating (2016): CiteScore 6.08
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 6
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 5.79
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 6.01
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 5.8
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Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 5.86
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Web of Science (2008): Indexed yes
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Supramolecular Derivation of Graphene Nanomaterials for Chemical Sensors

With properties such as high surface area, high conductivity, and low production cost with easy up-scaling, graphene-like materials provide a promising support for many applications, one of which is for chemical sensors. By functionalization with molecular receptors such as supramolecular moieties, which have long been used for chemical sensing, graphene-like materials can be endowed with increasing selectivity to form better and cheaper sensing composite materials.

In this Ph.D. project, reduced graphene oxide (RGO) has been covalently functionalized with supramolecular moieties to create active sensing materials. Two different strategies have been applied to achieve specific functionalization: The first approach consisted of covalently attaching chemically resistant supramolecular moieties, in the present work crown-ethers to graphene oxide (GO); the functionalized GO was then reduced chemically. This resulted in monolayer RGO nanosheets functionalized with crown-ether to an extent of up to 30% of the theoretically available surface area (Figure 1). These materials were shown to selectively bind alkali metal ions, and potentiometric sensing based on the materials was achieved with a detection limit of $10^{-5}$ M.

In the second approach Azido-RGO was prepared as a general platform for post reduction modification. GO was here functionalized with a short linker terminated in an alcohol. The intermediate material was then reduced effectively with NaBH₄, followed by chemical transformation of the alcohol into azide, thus providing a chemical handle for click chemistry in the form of CuAAC (Figure 2).

This platform material has then functionalized with ferrocene as a redox probe to accurately determine surface coverage which showed that the material one azido-functionality was attached per 16 RGO-sheet carbon atoms or slightly more than one azide per nm² of RGO-sheet.

This Azido-RGO was used in successful functionalization with the large supramolecular receptor molecules TTF-calix[4]pyrrole which function as a sensor for Cl⁻ and potentially for TNB. The coverage achieved was one molecule per 50 – 60 carbon atoms in the RGO-sheet. In view of the size of this molecular moiety, the coverage is actually very high. The material was used for Cl⁻ sensing showing sensitivity at very low concentration with linear response in the concentration range $10^{-6}$ – $10^{-5}$ M.
Synergy Effects of the Mixture of Bismuth Molybdate Catalysts with SnO2/ZrO2/MgO in Selective Propene Oxidation and the Connection between Conductivity and Catalytic Activity

Bismuth molybdate catalysts have been used for partial oxidation and ammoxidation of light hydrocarbons since the 1950s. In particular, there is the synergy effect (the enhancement of the catalytic activity in the catalysts mixed from different components) in different phases of bismuth molybdate catalysts which has been observed and studied since the 1980s; however, despite it being interpreted differently by different research groups, there is still no decisive conclusion on the origin of the synergy effect that has been obtained. The starting idea of this work is to find an answer for the question: does the electrical conductivity influence the catalytic activity (which has been previously proposed by some authors). In this work, highly conductive materials (SnO2, ZrO2) and nonconductive materials (MgO) are added to beta bismuth molybdates (beta-Bi2Mo2O9) using mechanical mixing, impregnation, and sol-gel methods. The mixtures were characterized by XRD, BET, XPS, and EDX techniques to determine the phase composition and surface properties. The conductivities of these samples were recorded at the catalytic reaction temperature (300-450 degrees C). Comparison of the catalytic activities of these mixtures showed that the addition of 10% mol SnO2 to beta bismuth molybdate resulted in the highest activity while the addition of nonconductive MgO could not increase the catalytic activity. This shows that there may be a connection between conductivity and catalytic activity in the mixtures of bismuth molybdate catalysts and other metal oxides.
Synthesis, Characterization and Evaluation of Tin-containing Silicates for Biomass Conversion

The transition to renewable carbon sources such as biomass will require entirely new catalytic processes and result in completely new products. An entire industry is built up around the chemicals that are available from fossil resources but will be unfeasible to prepare from other carbon sources. This dissertation describes the preparation and use of several important stannosilicate materials, known to transform carbohydrates into different valuable products. Several aspects of the tin-containing catalysts are investigated and discussed and new insight into the conversion of sugars is provided. The catalyst Sn-Beta is an important and highly active catalyst in a number of reactions. By carefully investigating the fluoride-route synthesis, the active component tin was discovered to influence the crystal morphology by changing the growth of the crystals. Even a small increase in tin content lead to much longer crystallization times (up to 60 days). Tin was furthermore not evenly distributed within the crystals, but instead found as an enriched outer shell. Small amounts of alkali were found to limit the growth retardation, enabling the preparations of Sn-Beta materials with high tin content.

For the catalytic conversion of sugars, the addition of alkali to the reaction media was also found to have a large effect on the product distribution. Having small concentrations of alkali present modified Sn-Beta to favor retro-aldol/aldol condensation reactions resulting in up to 75% methyl lactate from sucrose at optimized conditions. The effect of alkali was found to transcend to a variety of sugars, solvents and other stannosilicates such as Sn-MCM-41 or Sn-Beta prepared by a post-synthesis methodology. The latter makes it possible to use industrially relevant tin-containing catalysts to achieved high yields of methyl lactate simply by optimizing the amount of cosolute. In the absence of alkali, instead of retro-aldol reaction, hexoses and pentoses were found to undergo β-dehydration leading to several new and highly functional products. These include the trans-2,5,6-trihydroxy-3-hexenoic acid methyl ester (from hexoses) or trans-2,5-dihydroxy-3-pentenoic acid methyl ester (from pentoses) in acceptable yields (18-33%). Several additional products and intermediates were identified and quantified, providing a better understanding of the transformation of sugars catalyzed by tin. By using a zeolite with narrow channels (Sn-MFI), shape selectivity could be exploited for the valorization of small sugars. Glycolaldehyde (GA) could selectively undergo aldol condensation to give high yields of the rare tetroses (74%). With larger pore systems and channels either substantial yields of hexoses were formed from subsequent condensation reactions (Sn-MCM-41 and Sn-Beta): In the particular case of Sn-MFI and Sn-Beta, additional conversion of the tetroses lead to vinyl glycolic acid and α-hydroxy-γ-butyrolactone (HBL). Changing the conditions, it was possible to form up to 44% of VGA directly from GA using Sn-MFI. An important part of making the transition to more renewable resources is to have attractive alternatives to switch to. This means new, interesting chemicals easily obtainable from the most abundant biomass-derived sugars need to be found. The findings and processes investigated and discussed here should be a move in this direction.
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.
Synthesis of oligo (1→5)-α-L-arabinofuranosides related to the plant polysaccharide pectin

A strong fundamental understanding of plant biology is essential for meeting society’s growing demand for safe and nutritious food, dietary fibers, clothes, and renewable energy sources for an increasing global population. The plant cell wall is one of the main targets for biotechnological research, as it represents almost 50% of plant biomass.

A major constituent of the plant cell wall is different complex polysaccharides. The knowledge about their detailed structure and function on a molecular level is far from complete, and structural studies are complicated by the great complexity of the cell wall. The diversity of polysaccharides and the microheterogeneity in the cell wall make it extremely challenging to isolate well-defined compounds after partial degradation of plant material. Chemical synthesis, on the other hand, is capable of producing structurally diverse oligosaccharides of excellent purity, and in larger quantities.

The objective of the present study is to design and execute chemical syntheses of well-defined pectic oligosaccharides. These can serve as models for the more complex polysaccharide network found in the plant cell wall. The chemical synthesis of two branched structures of oligo (1→5)-α-L-arabinofuranosides that are prominent side chains in RG-I is presented. By employing a disaccharide donor, the number of glycosylation reactions was reduced significantly and late stage regioselective deprotection made it possible to introduce different sidechains in the oligosaccharides.

The work done during an external research stay at University of Copenhagen is also described. This includes the implementation of a covalent linker system as an alternative to bovine serum albumin (BSA) for oligosaccharides, as well as the development of a microarray-based transglycosylation assay capable of screening for novel glycosyl transferase/hydrolase activities.

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry
Authors: Daugaard, M. (Intern), Clausen, M. H. (Intern)
Synthesis of S-linked cellulose-oligosaccharides

Plant cell walls represent almost 50% of the biomass found in plants and therefore constitute one of the main targets for biotechnological research. For this reason, the transition to a sustainable bio-resource for future energy can primarily be founded on plant cell walls. Thus, in order to achieve a sustainable development, it is necessary to optimize plant production and its utilization. The polysaccharides present in the plant cell wall vary depending on the plant species and change during the developmental stage of the plant. As a result, this makes it very challenging to address the function of each individual component. The conversion of lignocellulosic biomass still remains a big challenge nowadays with the enzymatic hydrolysis being the limiting step. Indeed, characterization of the enzymes involved in this process can help the optimization development. For this reason, structurally well-defined oligosaccharides made via chemical synthesis can be used as models for the more complex polysaccharides in the investigation of properties such as polysaccharide biosynthesis, degradation and protein-carbohydrate interactions. For this purpose, non-natural substrate analogues forming irreversible binding to the enzyme can be employed. Thio-oligosaccharides represent the largest class of specific non-natural inhibitors for glycanases. In this thesis the chemical synthesis of some thio-glucans is presented. The formation of thio-linkages using a classical and non-classical method is investigated. Two strategies, relying on either a linear or a convergent strategy, have been employed in the synthesis towards two target molecules. Furthermore, the activity of a glycosyltransferase responsible for the elongation of a pectic polysaccharide has been investigated and partially characterized.

Synthesis of S-linked oligoxylans

The transition from a petroleum-dependent economy to one based on sustainable bio-resources will largely be founded on plant cell walls, as these are the largest source of biomass on earth. However, the development of lignocellulosic biomass conversion to fine chemicals and polymers still remains a big challenge for the biofuel industry. In particular, the enzymatic hydrolysis of lignocellulosic polysaccharides is one of the limiting steps of the entire procedure and therefore the enzymes involved in the degradation process must ideally be characterized and understood. This requires a detailed understanding of cell wall polysaccharide composition and architecture. Hemicelluloses are the second most abundant polymers in lignocellulosic biomass. They include different types of polysaccharides like xyloglucans, xylans, mannan, glucomannan and β-(1→3, 1→4)-glucans. Xylans are heteropolymers possessing a β-(1→4)-
Dxylopyranosebackbone, which is branched by short carbohydrate chains. The branches include D-glucuronic acid and its methyl ether, L-arabinose and/or various oligosaccharides like D-xylose, L-arabinose, D- or L-galactose and D-glucose. The hydrolysis of these polysaccharides is catalyzed by several families of enzymes, collected under the name of Glycosyl Hydrolases (GHs). Among other methods, the use of enzyme inhibitors like thio-linked oligosaccharides has for a long time been a common tool to analyze and characterize these enzymes. In the present work the chemical synthesis of thio-analogs of xylo- and arabinoxyloglycans is presented. Furthermore, the selection of a reliable method for the incorporation of thiolinkages in the synthesis of oligoxylans is also investigated. Therefore, different strategies for assembling S-linked disaccharides have been approached both involving 1-thioglycoside donors and thioacceptors. Advantages and disadvantages concerning the different methods are described and evaluated in relation to the synthesis of linear and branched oligoxylans.

General information
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Organisations: Department of Chemistry, Organic Chemistry, Joint Bioenergy Institute
Authors: Bonora, B. (Intern), Clausen, M. H. (Intern), Scheller, H. V. (Ekstern)
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Synthesis of sp3-rich scaffolds for molecular libraries through complexity-generating cascade reactions
An efficient strategy for the synthesis of complex small molecules from simple building blocks is presented. Key steps of the strategy include tandem Petasis and Diels–Alder reactions, and divergent complexity-generating cyclization cascades from a key dialdehyde intermediate. The methodology is validated through the synthesis of a representative compound set, which has been used in the production of 1617 molecules for the European Lead Factory.

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry, EDELRIS, Nanyang Technological University
Authors: Flagstad, T. (Intern), Min, G. (Intern), Bonnet, K. (Ekstern), Morgentin, R. (Ekstern), Roche, D. (Ekstern), Clausen, M. H. (Intern), Nielsen, T. E. (Intern)
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Web of Science (2017): Indexed Yes
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Scopus rating (2016): CiteScore 3.39 SJR 1.363 SNIP 0.803
Web of Science (2016): Indexed yes
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Scopus rating (2015): SJR 1.41 SNIP 0.858 CiteScore 3.47
Synthesis of β-1,4-Linked Galactan Side-Chains of Rhamnogalacturonan I

The synthesis of linear- and (1→6)-branched-β-(1→4)-D-galactans, side chains of the pectic polysaccharide rhamnogalacturonan I is described. The strategy relies on iterative couplings of n-pentenyl disaccharides followed by a late stage glycosylation of a common hexasaccharide core. Reaction with a covalent linker and immobilization on NHS-modified glass surfaces allows for the generation of carbohydrate microarrays. The glycan arrays enables the study of protein-carbohydrate interactions in a high throughput fashion, here demonstrated with binding to mAbs and CBMs.

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry, University of Copenhagen
Tandem Mannich/Diels–Alder reactions for the synthesis of indole compound libraries

A tandem Mannich/Diels–Alder sequence for the synthesis of small-molecule libraries with an indolyl-octahydro-3\textsubscript{a},6-epoxy-isoidole core structure is demonstrated in this study. Representative diversification examples based on this scaffold were performed, and a library is being produced within the European Lead Factory (ELF) Consortium.

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry, EDELRIS
Authors: Wu, P. (Intern), Petersen, M. Å. (Intern), Petersen, R. (Intern), Flagstad, T. (Intern), Guilleux, R. (Ekstern), Ohsten Rasmussen, M. (Ekstern), Morgentin, R. (Ekstern), Nielsen, T. E. (Intern), Clausen, M. H. (Intern)
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Scopus rating (2016): CiteScore 3.06 SJR 0.875 SNIP 0.743
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.959 SNIP 0.837 CiteScore 3.42
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.114 SNIP 0.965 CiteScore 3.87
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.117 SNIP 0.903 CiteScore 3.74
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Web of Science (2013): Indexed yes
Scopus rating (2012): SJR 0.863 SNIP 0.603 CiteScore 2.4
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The Au-S bond and SAM-protein contact in long-range electron transfer of pure and biomimetic metalloproteins via functionalized alkanethiol linkers

Interfacial electrochemical electron transfer (ET) of redox metalloproteins is long established. For the proteins to retain full ET or enzyme activity, modification of the electrode surfaces, say gold surfaces by self-assembled molecular monolayers (SAMs) is nearly always needed, where functionalized alkanethiols have emerged as core linkers. We have studied molecular linking in the long-range ET (LRET) processes in detail using electrochemistry, in situ STM and AFM, and electronic structure computations. A focus is the electronic structure of the Au-S link and the SAM packing. We have disentangled a wealth of data to identify the nature of the crucial Au-S contact, all suggesting prevalence of a Au(0)-thiyl radical unit. Molecular packing is further determined by the SAM molecular structure and involves binding either to Au-atoms mined out of the surface or directly to a flat surface. We illustrate this by high-resolution in situ STM of straight, branched, and chiral alkanethiols on Au(111)-electrode surfaces. We discuss next LRET of two SAM immobilized multi-copper enzymes, nitrite reductase and laccase, mapped to single-molecule resolution by in situ STM and AFM. The voltammetry is exceedingly sensitive to the structure of the thiol-based SAM molecules, testifying to the crucial importance of SAM packing and Au-S binding, and of the SAM link to the protein. Some of the subtleties are illustrated simpler by similar size (5-6 nm) nanoparticles (NPs). Biomimetic NPs must possess a certain degree of electronic structure sophistication. At the molecular scale this requirement is met by NPs of the renowned mixed-valence Prussian blue (PB) assembled on Au(111)-electrode surfaces via functionalized alkanethiols. PBNP SAMs show LRET comparable to metalloproteins. Alkanethiols with different terminal groups exhibit, further intriguing LRET differences, reflecting other subtleties. We discuss the molecular LRET mechanisms and the intrinsic conductivity of the PBNPs.

General information
State: Published
Organisations: Department of Chemistry, NanoChemistry, Organic Chemistry, UTS University of Technology Sydney, University of Sydney
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The crystal structure of human dopamine β-hydroxylase at 2.9 Å resolution

The norepinephrine pathway is believed to modulate behavioral and physiological processes, such as mood, overall arousal, and attention. Furthermore, abnormalities in the pathway have been linked to numerous diseases, for example hypertension, depression, anxiety, Parkinson’s disease, schizophrenia, Alzheimer’s disease, attention deficit hyperactivity disorder, and cocaine dependence. We report the crystal structure of human dopamine β-hydroxylase, which is the enzyme converting dopamine to norepinephrine. The structure of the DOMON (dopamine β-monooxygenase N-terminal) domain, also found in >1600 other proteins, reveals a possible metal-binding site and a ligand-binding pocket. The catalytic core structure shows two different conformations: an open active site, as also seen in another member of this enzyme family [the peptidylglycine α-hydroxylating (and α-amidating) monooxygenase], and a closed active site structure, in which the two copper-binding sites are only 4 to 5 Å apart, in what might be a coupled binuclear copper site. The dimerization domain adopts a conformation that bears no resemblance to any other known protein structure. The structure provides new molecular insights into the numerous devastating disorders of both physiological and neurological origins associated with the dopamine system.

General information
State: Published
Organisations: Department of Chemistry, X-ray Crystallography, Metalloprotein Chemistry and Engineering, Organic Chemistry, University of Oxford
Authors: Vendelboe, T. V. (Intern), Harris, P. (Intern), Zhao, Y. (Ekstern), Walter, T. S. (Ekstern), Harlos, K. (Ekstern), El Omari, K. (Ekstern), Christensen, H. E. M. (Intern)
It has been shown that certain N-aryltrichromethanesulfenamides Cl₃C-S-NHAr can be dehydrochlorinated to form red-colored thiocarbonyl S-imides CCl₂=S=NR which dimerize spontaneously. The dimers so far obtained were first assigned the 1,4,2,5-dithiadiazinane structure but later shown to be the isomeric 1,4,2,3-dithiadiazinanes. It is proposed that both the so far unknown 1,4,2,5-dithiadiazinanes and the so far elusive thiocarbonyl S-imides (RRC)-R-1-C-2=S=NR₃ might be made directly observable by introducing massive steric strain via bulky R in the starting chlorinated sulfenamides such as Cl₃C-S-NHAr and CCl₃CCl₂-S-NHR. According to PM7 and DFT type MO calculations of the enthalpies, the formation of the 1,4,2,5-dithiadiazinanes is thermodynamically favored over that of the 1,4,2,3-isomers. However, the activation energies for the cyclization reaction are lower for the head-to-head dimerization. Thus, the observed dimerization of thiocarbonyl S-imides under formation of 1,4,2,3-dithiadiazinanes is a kinetically controlled reaction.
The donor OH stretching-libration dynamics of hydrogen-bonded methanol dimers in cryogenic matrices

FTIR spectra of the methanol dimer trapped in neon matrices are presented. The fundamental, overtone and combination bands involving the donor OH libration and stretching motions were observed in order to extract relevant anharmonicity constants. We find a stretching-libration coupling constant of $+43(5)$ cm$^{-1}$ and a diagonal librational anharmonicity constant of $-71(5)$ cm$^{-1}$. The spectra are compared to a number of VPT2 calculations and a torsionally localized monomer model in order to enhance previous explanations of the observable OH stretching red-shift upon dimerization.

General information
State: Published
Organisations: Department of Chemistry, University of Göttingen
Authors: Heger, M. (Ekstern), Andersen, J. (Intern), Suhm, M. A. (Ekstern), Larsen, R. W. (Intern)
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Main Research Area: Technical/natural sciences

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The dynamic mechanism of presenilin-function: Sensitive gate dynamics and loop unplugging control protein access

There is no molecular explanation for the many presenilin 1 (PSEN1) mutations causing Alzheimer's disease, but both gain of function relating to amyloid production and loss of isolated PSEN1 function have been implied. We report here the first detailed dynamic all-atom model of mature PSEN1 from molecular dynamics in an explicit membrane with particular account of the as yet unexplored loop dynamics. We find that mature PSEN1 contains multiple distinct conformational states whereas non-mature PSEN1 is a typical one-state protein. We confirm a previously suggested gating mechanism, and find that the 106-131 loop acts as a "hinge" for the TM2 and TM6 "doors". More importantly, we identify an unplugging mechanism of the Exon 9 loop associated only with mature PSEN1. Proper opening of both the "gate" and "plug" in the membrane produces channel-like morphologies and access to the catalytic aspartates. Dynamically, these features seem linked. The long-range sensitivity of this gate-plug system to subtle conformational changes can explain why so many PSEN1 mutants cause disease. Reduced access and imprecise substrate cleavage associated with impaired gate-plug dynamics is directly illustrated by the effect of maturation in our work and could explain the overall reduction in Aβ levels upon PSEN1 mutation and the increase in the Aβ 42/40 ratio. Yet, our PSEN1-only dynamics are particularly insightful in revealing PSEN1-only dynamics relating to e.g. its role as membrane channel. Thus, our identified gate-plug mechanism is relevant for designing PSEN1 modulating therapies for treatment of Alzheimer's disease within both the amyloid/γ-secretase hypothesis and within the PSEN1 loss of function paradigm.
The Impact of Strong Cathodic Polarization on SOC Electrolyte Materials

One of the most promising reversible energy conversion/storage technologies is that of Solid Oxide Fuel/Electrolysis Cells (SOFC/SOEC, collectively termed SOC). Long term durability is typically required for such devices to become economically feasible, hence considerable amount of work has and is being done on the degradation and long term durability of these systems. When using a SOC in electrolysis mode, it is economically beneficial to operate the cell at high current density, since it increases the fuel production rate. However, several degradation phenomena, such as segregation of impurities at the grain boundaries, electrode poisoning, delamination or cracks of the electrolyte etc., have been observed in cells operated at such conditions, lowering the lifetime of the cell1,2. High polarizations are observed at the electrolyte/cathode interface of an electrolysis cell operated at high current density. In case of a cell voltage above 1.6 V, p-type and n-type electronic conductivity are often observed at the anode and cathode respectively3. Hence, a considerable part of the current is lost as leakage through the electrolyte, thus lowering the efficiency of the cell considerably.

The Importance of Magnesium in the Human Body: A Systematic Literature Review

Magnesium, the second and fourth most abundant cation in the intracellular compartment and whole body, respectively, is of great physiologic importance. Magnesium exists as bound and free ionized forms depending on temperature, pH, ionic strength, and competing ions. Free magnesium participates in many biochemical processes and is most commonly
measured by ion-selective electrode. This analytical approach is problematic because complete selectivity is not possible
due to competition with other ions, i.e., calcium, and pH interference. Unfortunately, many studies have focused on
measurement of total magnesium rather than its free bioactive form making it difficult to correlate to disease states. This
systematic literature review presents current analytical challenges in obtaining accurate and reproducible test results for
magnesium.

The Influence of Conjugated Polymer Side Chain Manipulation on the Efficiency and Stability of Polymer Solar Cells

The stability of polymer solar cells (PSCs) can be influenced by the introduction of particular moieties on the conjugated
polymer side chains. In this study, two series of donor-acceptor copolymers, based on bis(thienyl)dialkoxybenzene donor
and benzo[c][1,2,5]thiadiazole (BT) or thiazolo[5,4-d]thiazole (TzTz) acceptor units, were selected toward effective device
scalability by roll-coating. The influence of the partial exchange (5% or 10%) of the solubilizing 2-hexyloxyethoxy by
alternative 2-phenylethoxy groups on efficiency and stability was investigated. With an increasing 2-phenylethoxy ratio, a
decrease in solar cell efficiency was observed for the BT-based series, whereas the efficiencies for the devices based on
the TzTz polymers remained approximately the same. The photochemical degradation rate for PSCs based on the TzTz
polymers decreased with an increasing 2-phenylethoxy ratio. Lifetime studies under constant sun irradiance showed a
diminishing initial degradation rate for the BT-based devices upon including the alternative side chains, whereas the (more
stable) TzTz-based devices degraded at a faster rate from the start of the experiment upon partly exchanging the side
chains. No clear trends in the degradation behavior, linked to the copolymer structural changes, could be established at
this point, evidencing the complex interplay of events determining PSCs’ lifetime.
Fluorinated phospholipid analogues are investigated as potential substrates for phospholipase A(2) (PLA(2)) using classical molecular dynamics simulations and quantum mechanics/density functional theory calculations. The fluorinated phospholipid analogues are α-fluoro (HF-ProAEL) and α,α-difluoro (F-2-ProAEL) conjugates of (R)-1-O-hexadecyl-2-palmitoyl-sn-glycero-3-phosphocholineglycerol (ProAEL). Our results provide a theoretical assessment of the potential usefulness of these fluorinated lipids in the rational design of liposomal drug-delivery systems. The α-fluorine-substituted phospholipid analogues are found to be substrates for secretory PLA(2), with sufficient accessibility of water to the active site to allow for enzymatic hydrolysis. Because of the inherently less stable nature of HF-ProAEL and F-2-ProAEL when compared to that of ProAEL, the hydrolytic reaction is predicted to occur at a progressively faster rate; the more electronegative substituent at the α-position effectively lowers the energy barrier for hydrolysis. We conclude that the partially fluorinated phospholipid analogues facilitate rational design of liposomal vesicles of phospholipid mixtures with desirable physicochemical properties and that are still subjects for important and pharmaceutically proven drug-delivery mechanisms.
Theoretical Study of Spin Crossover in 30 Iron Complexes

Spin crossover was studied in 30 iron complexes using density functional theory to quantify the direction and magnitude of dispersion, relativistic effects, zero-point energies, and vibrational entropy. Remarkably consistent entropy–enthalpy compensation was identified. Zero-point energies favor high-spin by 9 kJ/mol on average; dispersion and relativistic effects both favor low-spin by 9 kJ/mol on average. These drivers dominate the thermodynamics (but not the transition nature) of SCO and should be considered in rational design of new spin crossover systems.
The Phase Envelope of Multicomponent Mixtures in the Presence of a Capillary Pressure Difference

Confined fluids such as oil and gas mixtures inside tight reservoirs are systems that can experience high capillary pressure difference between the liquid and gas phases. This capillary pressure difference has an effect on the phase equilibrium and in some cases is considerably high. We presented an algorithm which can reliably compute the whole phase envelope for multicomponent mixtures when there is a capillary pressure difference. It uses an equation of state for the phase equilibrium and the Young-Laplace equation for the capillary pressure model. The algorithm proves to be robust and efficient for test mixtures with wide ranges of compositions at different capillary radii and vapor fractions. The calculation results show that the phase envelope changes everywhere except at the critical point. The bubble point and the lower branch of the dew point show a decrease in the saturation pressure, whereas the upper branch of the dew point shows an increase. The cricondentherm is shifted to a higher temperature. We also presented a mathematical analysis of the phase envelope shift due to capillary pressure based on linear approximations. The resulting linear approximation equations can predict the correct direction of the phase envelope shift. Combined with the multicomponent Clapeyron equation, the equations reveal why the shift changes direction for the saturation pressure at the cricondentherm and for the saturation temperature at the cricondenbar. The equations can be used to estimate the magnitude of shift, and the approximation is close for the change in the bubble point pressure.

General information
State: Published
Organisations: Center for Energy Resources Engineering, Department of Chemistry, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering
Authors: Sandoval Lemus, D. R. (Intern), Yan, W. (Intern), Michelsen, M. L. (Intern), Stenby, E. H. (Intern)
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BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.1 SJR 0.945 SNIP 1.139
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.949 SNIP 1.146 CiteScore 2.87
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.012 SNIP 1.292 CiteScore 2.85
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Tin-Containing Silicates: Identification of a Glycolytic Pathway via 3-Deoxyglucosone

Inorganic glycolytic systems, capable of transforming glucose through a cascade of catalytic steps, can lead to efficient chemical processes utilising carbohydrates as feedstock. Tin-containing silicates, such as Sn-Beta, are showing potential for the production of lactates from sugars through a cascade of four to five sequential steps. Currently, there is a limited understanding of the competing glycolytic pathways within these systems. Here we identify dehydration of glucose to 3-deoxyglucosone as an important pathway that occurs in addition to retro-aldol reaction of hexoses when using tin-containing silicates. It is possible to influence the relative carbon flux through these pathways by controlling the amount of alkali metal salts present in the reaction mixture. In the absence of added potassium carbonate, at least 15–30% carbon flux via 3-deoxyglucosone is observed. Addition of just a few ppm of potassium carbonate makes retro-aldol pathways dominant and responsible for about 60–70% of the overall carbon flux. The 3-deoxyglucosone pathway results in new types of chemical products accessible directly from glucose. Furthermore, it is argued that 3-deoxyglucosone is a
contributing source of some of the methyl lactate formed from hexoses using tin-containing silicates in the presence of alkali metal salts. Further catalyst design and system tuning will permit even better control between these two different glycolytic pathways and will enable highly selective catalytic transformations of glucose to a variety of chemical products using tin-containing silicates.

**General information**

State: Published

Organisations: Department of Chemistry, Organic Chemistry, Centre for Catalysis and Sustainable Chemistry, Aarhus University, Haldor Topsoe AS

Authors: Tolborg, S. (Intern), Meier, S. (Intern), Sádaba, I. (Ekstern), Elliot, S. G. (Intern), K. Kristensen, S. (Ekstern), Shunmugavel, S. (Intern), Riisager, A. (Intern), Fristrup, P. (Intern), Skrydstrup, T. (Ekstern), Taarning, E. (Ekstern)

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BFI (2016): BFI-level 2

Scopus rating (2016): CiteScore 8.86 SJR 2.564 SNIP 2.019

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

Scopus rating (2007): SJR 2.129 SNIP 1.554

Web of Science (2007): Indexed yes

Scopus rating (2006): SJR 1.539 SNIP 1.414

Web of Science (2006): Indexed yes
Towards the Synthesis of Carrageenan Oligosaccharides

The plant cell walls represent almost 50% of the biomass found in plants and are therefore one of the main targets for biotechnological research. Many of their components already have important industrial applications in various fields, such as in the food and biomedical industry and in biofuel production. Therefore, it is necessary to optimize the plant production and its utilization. This will require a better understanding of the cell wall structure and function at the molecular level. Most of the studies achieved on plant cell wall structures and their biosynthesis have been focusing on land plants. Only very few reports are dealing with algae. However, land plants have algae ancestors and getting a better knowledge of algae cell walls could help understand the evolution of plant cell walls. Furthermore, some components specific to algae cell walls are very valuable in the industry. Indeed, the polysaccharides present in the plant cell wall vary depending on the plant species and change during the developmental stage of the plant. This makes it very challenging to address the function of individual components in living cells as well as study the physical properties of each particular molecule. Alternatively, structurally defined oligosaccharides can be used as models for the more complex polysaccharide components. This would enable to investigate a range of properties such as cell wall biosynthesis and protein-carbohydrate interactions, but also the physical properties of the pure oligosaccharides in order to optimize their applications in the industry. Chemical or enzymatic degradation of plant cell wall can provide some oligosaccharides but extensive purification is required and only a limited range of structures has so far been isolated. Chemical synthesis, on the other hand, is capable of producing structurally diverse oligosaccharides of excellent purity and in higher quantities. This thesis presents the development of a synthetic strategy to produce ten different types of carrageenan oligosaccharides from one single precursor. These molecules are highly sulfated galactans, which are found in the cell wall of red algae and serve as gelling, stabilizing and viscosity-enhancing agents in many sectors ranging from the food industry to pharmaceuticals. A modular approach was chosen to enable the synthesis of carrageenan oligosaccharides with different lengths. Different protecting group patterns were tested to synthesize the oligosaccharide backbone. A protected tetrasaccharide precursor was synthesized and can be used to synthesize all ten carrageenan tetrasaccharides. Optimization of the deprotection steps as well as sulfation was done on a similar disaccharide and one disaccharide carrageenan was synthesized in the end. These steps were further translated successfully to the desired tetrasaccharide. A work dealing with the development of an intramolecular catalyzed fluoroarylation is presented at the end of this thesis. A range of different allyl substituted aryl boronic acids substrates were synthesized in order to investigate the scope of a silver catalyzed reaction and some preliminary results of the catalytic reaction are presented.
Tracking evolution of myoglobin stability in cetaceans using experimentally calibrated computational methods that account for generic protein relaxation

The evolution of cetaceans (whales, dolphins, and porpoises) from land to water is one of the most spectacular events in mammal evolution. It has been suggested that selection for higher myoglobin stability (ΔG of folding) allowed whales to conquer the deep-diving niche. The stability of multi-site protein variants, including ancient proteins, is however hard to describe theoretically. From a compilation of experimental ΔΔG vs. ΔG we first find that protein substitutions are subject to large generic protein relaxation effects. Using this discovery, we develop a simple two-parameter model that predicts multi-site ΔΔG as accurately as standard methods do for single-site mutations and reproduces trends in contemporary myoglobin stabilities. We then apply this new method to the study of the evolution of Mb stability in cetaceans: With both methods the main change in stability (about 1 kcal/mol) occurred very early, and stability was later relaxed in dolphins and porpoises, but was further increased in the sperm whales. This suggests that single proteins can affect whole organism evolution and indicates a role of Mb stability in the evolution of cetaceans. Transition to the deep-diving niche probably occurred already in the ancestor of contemporary baleen and toothed whales. In summary, we have discovered generic stability relaxation effects in proteins that, when incorporated into a simple model, improves the description of multi-site protein variants.
Understanding degradation of solid oxide electrolysis cells through modeling of electrochemical potential profiles

Establishing the spatial distribution of the various chemical and electrochemical potentials in an operating SOEC is critical as several degradation mechanisms are tightly connected to them, but at the same time very challenging to achieve experimentally. Such distributions are presented here on the basis of a two dimensional bi-layer electrolyte SOC model including for both electrodes a description of activation, concentration, and conversion losses. An extensive parametric study is reported to illustrate the influence of the electrode polarization resistances, the ionic and electronic conductivities in the electrolyte, the gas composition, temperature, and pressure on the current density distribution over the cell and the oxygen activity distribution within the electrolyte. The developed model is further used to simulate long-term durability experiments during different stages of operation, thereby helping to rationalize microstructural and chemical changes observed in post-mortem analysis. Finally, measures to mitigate degradation by changing conditions of operation, material or electrode properties or overall cell geometry are suggested.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Fundamental Electrochemistry, Mixed Conductors, Department of Chemistry
Authors: Chatzichristodoulou, C. (Intern), Chen, M. (Intern), Hendriksen, P. V. (Intern), Jacobsen, T. (Intern), Mogensen, M. B. (Intern)
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Journal: Electrochimica Acta
Volume: 189
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BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.74 SJR 1.357 SNIP 1.167
Web of Science (2016): Indexed yes
Ruthenium PNP complex 1a (RuH(CO)Cl(HN(C$_2$H$_4$Pi-Pr$_2$)$_2$)) represents a state-of-the-art catalyst for low-temperature (<100 °C) aqueous methanol dehydrogenation to H$_2$ and CO$_2$. Herein, we describe an investigation that combines experiment, spectroscopy, and theory to provide a mechanistic rationale for this process. During catalysis, the presence of two anionic resting states was revealed, Ru–dihydride (3–) and Ru–monohydride (4–) that are deprotonated at nitrogen in the pincer ligand backbone. DFT calculations showed that O- and CH- coordination modes of methoxide to ruthenium
compete, and form complexes 4⁻ and 3⁻, respectively. Not only does the reaction rate increase with increasing KOH, but the ratio of 3⁻/4⁻ increases, demonstrating that the "inner-sphere" C—H cleavage, via C—H coordination of methoxide to Ru, is promoted by base. Protonation of 3⁻ liberates H₂ gas and formaldehyde, the latter of which is rapidly consumed by KOH to give the corresponding gem-diolate and provides the overall driving force for the reaction. Full MeOH reforming is achieved through the corresponding steps that start from the gem-diolate and formate. Theoretical studies into the mechanism of the catalyst Me-1a (N-methylated 1a) revealed that C—H coordination to Ru sets-up C—H cleavage and hydride delivery; a process that is also promoted by base, as observed experimentally. However, in this case, Ru–dihydride Me-3 is much more stable to protonation and can even be observed under neutral conditions. The greater stability of Me-3 rationalizes the lower rates of Me-1a compared to 1a, and also explains why the reaction rate then drops with increasing KOH concentration.

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Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry, University of Rostock, CreativeQuantum GmbH
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Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 13.18 SJR 7.368 SNIP 2.584
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 6.826 SNIP 2.632 CiteScore 12.81
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 6.273 SNIP 2.578 CiteScore 11.92
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 5.953 SNIP 2.455 CiteScore 11.38
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 6.141 SNIP 2.379 CiteScore 10.37
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 5.447 SNIP 2.336 CiteScore 9.94
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 5.076 SNIP 2.132
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 4.883 SNIP 2.176
The role played by quantum interference in the laser phase modulation coherent control of photofragment distributions in the weak-field regime is investigated in detail in this work. The specific application involves realistic wave packet calculations of the transient vibrational populations of the Br$_2$(B,vf) fragment produced upon predissociation of the Ne-Br$_2$(B) complex, which is excited to a superposition of overlapping resonance states using different fixed bandwidth pulses where the linear chirps are varied. The postpulse transient phase modulation effects observed on fragment populations for a long time window are explained in terms of the mechanism of interference between overlapping resonances. A detailed description of how the interference mechanism affects the magnitude and the time window of the phase control effects is also provided. In the light of the results, the conditions to maximize phase modulation control on fragment distributions are discussed.

Unravelling the role of quantum interference in the weak-field laser phase modulation control of photofragment distributions

General information
State: Published
Organisations: Department of Chemistry, Consejo Superior de Investigaciones Científicas
Authors: García-Vela, A. (Ekstern), Henriksen, N. E. (Intern)
Number of pages: 8
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Journal: Physical Chemistry Chemical Physics
Volume: 18
Issue number: 6
ISSN (Print): 1463-9076
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BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
Voltammetry and Molecular Assembly of G-quadruplex DNAzyme on Single-crystal Au(111)-electrode Surfaces – Hemin as an Electrochemical Intercalator

DNA quadruplexes (qs’s) are a class of “non-canonical” oligonucleotides (OGNs) composed of stacked guanine (G) quartets generally stabilized by monovalent cations. Metal porphyrins selectively bind to G-qs complexes to form DNAzyme, which can exhibit peroxidase and other catalytic activity similar to heme group metalloenzymes. In the present study we investigate the electrochemical properties and the structure of DNAzyme monolayers on single-crystal Au(111)-electrode surfaces using cyclic voltammetry and scanning tunnelling microscopy under electrochemical potential control (in situ STM). The target DNZyme is formed from a single-strand OGN with 12 guanines and iron (III) porphyrin IX (hemin), and assembles on Au(111) by the mercapto alkyl linker. The DNAzyme monolayers exhibit a strong pair of redox peaks at 0.0 V (NHE) at pH 7 in acetate buffer, shifted positively by about 50 mV compared to free hemin physisorbed on the Au(111). The voltammetric signal of DNZyme is enhanced 15 times, indicative that hemin is strongly bound to the immobilized 12G-qs and in well-defined orientation favorable for interfacial ET with a rate constant of 6.0 s−1. The G-quartet structures with a size of 1.6 ± 0.2 nm are observed under in situ STM.

General information
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Organisations: Department of Chemistry, NanoChemistry, Organic Chemistry
Authors: Zhang, L. (Intern), Ulstrup, J. (Intern), Zhang, J. (Intern)
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.07 SJR 1.504 SNIP 0.925
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.51 SNIP 1.051 CiteScore 3.54
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.7 SNIP 1.278 CiteScore 3.79
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.618 SNIP 1.12 CiteScore 3.65
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.732 SNIP 0.948 CiteScore 3.24
ISI indexed (2012): ISI indexed no
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.893 SNIP 1.239 CiteScore 3.92
ISI indexed (2011): ISI indexed no
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.719 SNIP 1.22
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.799 SNIP 1.157
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.792 SNIP 1.293
Water vapor pressure over molten KH₂PO₄ and demonstration of water electrolysis at ∼300°C

A new potentially high-efficiency electrolyte for water electrolysis: molten monobasic potassium phosphate, KH₂PO₄ or KDP has been investigated at temperatures ~275–325 °C. At these temperatures, KH₂PO₄ was found to dissociate into H₂O gas in equilibrium with a melt mixture of KH₂PO₄—K₂H₂P₂O₇—KPO₃—H₂O. The water vapor pressure above the melt, when contained in a closed ampoule, was determined quantitatively vs. temperature by use of Raman spectroscopy with methane or hydrogen gas as an internal calibration standard, using newly established relative ratios of Raman scattering cross sections of water and methane or hydrogen to be 0.40 ± 0.02 or 1.2 ± 0.03. At equilibrium the vapor pressure was much lower than the vapor pressure above liquid water at the same temperature. Electrolysis was realized by passing current through closed ampoules (vacuum sealed quartz glass electrolysis cells with platinum electrodes and the electrolyte melt). The formation of mixtures of hydrogen and oxygen gases as well as the water vapor was detected by Raman spectroscopy. In this way it was demonstrated that water is present in the new electrolyte: molten KH₂PO₄ can be split by electrolysis via the reaction 2H₂O → 2H₂ + O₂ at temperatures ~275–325 °C. At these temperatures, before the start of the electrolysis, the KH₂PO₄ melt gives off H₂O gas that pressurizes the cell according to the following dissociations: 2KH₂PO₄ ↔ K₂H₂P₂O₇ + H₂O ↔ 2KPO₃ + 2H₂O. The spectra show however that the water by virtue of hydrogen-bonding has a high affinity for remaining in the melt. The formed hydrogen and oxygen gasses were detected by means of the characteristic Raman gas-phase spectra.
Zeolite and zeotype-catalysed transformations of biofuranic compounds

Catalytic valorisation of biomass with solid functional materials has been recognised as a promising approach to produce value-added biochemicals and biofuels. Furanic compounds such as 5-hydroxymethylfurfural (HMF), 5-ethoxymethylfurfural, 2,5-dimethylfuran, 2,5-diformylfuran and 2,5-furandicarboxylic acid can be obtained from hexoses and pentoses via selective dehydration and subsequent etherification, hydrogenation, oxidation reactions, which show great potential for industrial applications to replace petroleum-based chemicals and fuels. Zeolite and zeotype micro- and mesoporous materials with tuneable acidity, good thermal stability and shape-selectivity have recently emerged as promising solid catalysts, exhibiting superior catalytic performance to other heterogeneous catalysts. This review focuses
on the synthesis of biomass-derived furanic compounds catalysed by zeolitic materials, firstly introducing zeolite-catalysed
dividuals- and oligo- and polysaccharides and isomerization reactions of monomeric sugars. Subsequently, the catalytic
dehydration reactions of hexoses and pentoses to obtain HMF and furfural are reported. Particularly, a variety of reaction
pathways towards upgrading of the resulting platform furanic molecules to valuable bioproducts over zeolitic materials are
discussed.

General information
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Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Guizhou University, Centre of
Innovative and Applied Bioprocessing, Universidad de Cordoba
Authors: Li, H. (Ekstern), Yang, S. (Ekstern), Riisager, A. (Intern), Pandey, A. (Ekstern), Sangwan, R. S. (Ekstern),
Saravanamurugan, S. (Ekstern), Luque, R. (Ekstern)
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BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 8.86 SJR 2.564 SNIP 2.019
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
Scopus rating (2007): SJR 2.129 SNIP 1.554
Web of Science (2007): Indexed yes
Zeolite-catalyzed conversion of sucrose to fructose

General information
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Organisations: Centre for Catalysis and Sustainable Chemistry, Organic Chemistry, Department of Chemistry, Technical University of Denmark, Haldor Topsoe AS
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Links:
http://www.sustain.dtu.dk/

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

β-Amyloid pathogenesis: Chemical properties versus cellular levels

Although genetic Aβ variants cause early-onset Alzheimer's disease, literature reports on Aβ properties are heterogeneous, obscuring molecular mechanisms, as illustrated by recent failures of Aβ-level targeting trials. Thus, we combined available data on Aβ levels and ratios, aggregation propensities, toxicities, and patient data for Aβ variants and correlated these data to identify heterogeneity, significant relations, and basis for consensus. Despite heterogeneity, age of disease onset correlates to Aβ levels ($R^2 = 0.38, P = .018$), but not to toxicities, Aβ$_{42}$ levels, Aβ$_{42}$/Aβ$_{40}$ ratios, or aggregation propensities. Cytotoxicity correlates inversely with total Aβ$_{42}$ ($R^2 = 0.65, P = .016$) and Aβ$_{42}$/Aβ$_{40}$ ratios ($R^2 = 0.76, P = .005$), i.e., chemical properties that increase Aβ$_{42}$ also reduce toxicity. The complexity and heterogeneity of data reveal the need to understand these phenotypes better, e.g., by focusing on the chemical properties of the involved Aβ species.

General information
State: Published
Organisations: Department of Chemistry, Physical and Biophysical Chemistry
Authors: Tiwari, M. K. (Intern), Kepp, K. P. (Intern)
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Volume: 12
Issue number: 2
ISSN (Print): 1552-5260
Ratings:
Web of Science (2018): Indexed yes
Web of Science (2017): Indexed Yes
Method for the preparation of intermediates for carboxy-fluoresceins and novel carboxy-fluorescein.

The invention provides a method for the preparation of regioisomerically pure intermediates which are useful for the preparation of carboxy-fluorescein-type compounds. Such compounds have broad applications within bio-conjugation and/or fluorescent imaging.

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry
Authors: Hammershøj, P. L. (Ekstern), Clausen, M. H. (Intern)
Publication date: 12 Nov 2015

Publication information
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Patent number: WO2015169854
Date: 12/01/1915
Priority date: 26/03/2015
Priority number: EP20150161033
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Main Research Area: Technical/natural sciences
Source: espacenet
Source-ID: WO2015169854
Publication: Research › Patent – Annual report year: 2016

Combined oxidation and absorption of nox by an ionic liquid tandem process.

The present invention relates to a new strategy for capturing NOx using a two-step process.

General information
State: Published
Organisations: Department of Chemistry, Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry, DTU Admission Course, Office for Research and Relations, Risø National Laboratory for Sustainable Energy
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

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
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BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.55 SJR 0.974 SNIP 0.878
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
Scopus rating (2009): SJR 1.269 SNIP 0.907
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.225 SNIP 1.015
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.522 SNIP 1.382
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.59 SNIP 1.202
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.444 SNIP 1.17
Scopus rating (2004): SJR 1.374 SNIP 1.136
Scopus rating (2003): SJR 1.229 SNIP 0.915
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 1.233 SNIP 0.874
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 1.451 SNIP 1.087
Scopus rating (2000): SJR 2.482 SNIP 1.684
Web of Science (2000): Indexed yes
Co2 chemosorption by functionalized amino acid derivatives.
The absorption and desorption behaviour of carbon dioxide (CO2) using a composition comprising an ionic compound comprising a cation [A+] and an anion [B-] is described, wherein the anion [B-] is a mono-amine functionalized amino acid.

General information
State: Published
Organisations: Technical University of Denmark, Department of Chemistry, Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry
Authors: Fehrmann, R. (Intern), Riisager, A. (Intern), Shunmugavel, S. (Intern)
Publication date: 23 Jul 2015
A Method for Effective Conversion of Saccharides to Furfural Compounds
The present invention relates to a method for the effective conversion of one or more mono-, di-, oligo- or polysaccharides to hydroxymethylfurfural (HMF), in an ionic liquid by means of a chromium catalyst mixture comprising chromium (II) and chromium (III) species. The invention also provides a catalyst mixture suitable for this conversion.

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry, X-ray Crystallography, Centre for Catalysis and Sustainable Chemistry
Authors: Malcho, P. (Intern), Andersen, J. (Intern), Kunov-Kruse, A. J. (Intern), Ståhl, K. (Intern), Riisager, A. (Intern), Fehrmann, R. (Intern)
Publication date: 15 Jan 2015

Publication information
IPC: C07D307/50
Patent number: WO2015004273
Date: 15/01/2015
Priority date: 12/07/2013
Priority number: EP20130176259
Original language: English
Electronic versions:
WO2015004273A1.pdf

Bibliographical note
Also registered as: WO2014EP64942, EP20130176259
Main Research Area: Technical/natural sciences
Source-ID: WO2015004273
Publication: Research › Patent – Annual report year: 2015

The focus of this work is on the synthesis of a 1-Aza-18-crown[6]ether functionalized reduced graphene oxide (RGO-crown[6]) with specific K+ binding sites on the RGO surface. Glassy carbon electrodes (GCE) functionalized with RGO-crown[6] were tested for selective potentiometric sensing of K+, with a detection limit of $10^{-5}$ M without inference from other ions (Na+, Li+, NH4+ and Ca2+) in concentrations up to $2.5 \times 10^{-2}$ M. Similar sensing was achieved with functionalized disposable SPE electrodes. The results demonstrate that RGO-crown[6] is a conductive material full of promise for application in fabrication of new types of ion selective sensors.

General information
State: Published
Organisations: Department of Chemistry, NanoChemistry, Organic Chemistry
Authors: Olsen, G. (Intern), Ulstrup, J. (Intern), Chi, Q. (Intern)
Number of pages: 1
Publication date: 2015
Event: Poster session presented at 6th Symposium on Carbon and Related Nanomaterials, Copenhagen, Denmark.
Main Research Area: Technical/natural sciences
Electronic versions:
18_Crown_6_ether_functionalized_reduced_graphene.pdf
Source-ID: 118201738
Publication: Research - peer-review › Poster – Annual report year: 2015

3D Graphene-based bio-cathode for Carbon dioxide reduction in Microbial Electrosynthesis

General information
State: Published
Organisations: Novo Nordisk Foundation Center for Biosustainability, Research Groups, Bioelectrochemical Systems, Department of Chemistry, NanoChemistry, Organic Chemistry
Authors: Aryal, N. (Intern), Halder, A. (Intern), Tremblay, P. (Intern), Chi, Q. (Intern), Zhang, T. (Intern)
Number of pages: 1
Publication date: 2015
Acetaldehyde as an intermediate in the electroreduction of carbon monoxide to ethanol on oxide-derived copper

General information
State: Published
Organisations: Department of Physics, Experimental Surface and Nanomaterials Physics, Department of Chemistry, Organic Chemistry, Carlsberg Laboratory
Number of pages: 1
Publication date: 2015

A consistent reaction mechanism for the selective catalytic reduction of NO with NH₃

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry, Haldor Topsoe AS, University of Turin
Publication date: 2015
Event: Abstract from 249th ACS National Meeting & Exposition, Denver, CO, United States.
Main Research Area: Technical/natural sciences
Electronic versions: Abstract.pdf

Relations
Activities:
A consistent reaction mechanism for the selective catalytic reduction of NO with NH₃
Publication: Research › Conference abstract for conference – Annual report year: 2015

A consistent reaction scheme for the selective catalytic reduction of nitrogen oxides with ammonia
For the first time, the standard and fast selective catalytic reduction of NO by NH₃ are described in a complete catalytic cycle, that is able to produce the correct stoichiometry, while only allowing adsorption and desorption of stable molecules. The standard SCR reaction is a coupling of the activation of NO by O₂ with the fast SCR reaction, enabled by the release of NO₂. According to the scheme, the SCR reaction can be divided in an oxidation of the catalyst by NO + O₂ and a reduction by NO + NH₃; these steps together constitute a complete catalytic cycle. Furthermore both NO and NH₃ are required in the reduction, and, finally, oxidation by NO + O₂ or NO₂ leads to the same state of the catalyst. These points are shown experimentally for a Cu-CHA catalyst, by combining in situ X-ray absorption spectroscopy (XAS), electron
paramagnetic resonance (EPR), and Fourier transform infrared spectroscopy (FTIR). A consequence of the reaction scheme is that all intermediates in fast SCR are also part of the standard SCR cycle. The calculated activation energy by density functional theory (DFT) indicates that the oxidation of an NO molecule by O₂ to a bidentate nitrate ligand is rate determining for standard SCR. Finally, the role of a nitrate/nitrite equilibrium and the possible influence of Cu dimers and Brønsted sites are discussed, and an explanation is offered as to how a catalyst can be effective for SCR, while being a poor catalyst for NO oxidation to NO₂.

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Haldor Topsoe AS, University of Turin
Authors: Janssens, T. V. (Ekstern), Falsig, H. (Ekstern), Lundegaard, L. F. (Ekstern), Vennestrøm, P. N. R. (Ekstern), Rasmussen, S. B. (Ekstern), Moses, P. G. (Ekstern), Giordanino, F. (Ekstern), Borfecchia, E. (Ekstern), Lomachenko, K. A. (Ekstern), Lamberti, C. (Ekstern), Bordiga, S. (Ekstern), Godiksen, A. (Intern), Mossin, S. (Intern), Beato, P. (Ekstern)
Number of pages: 14
Pages: 2832-2845
Publication date: 2015
Main Research Area: Technical/natural sciences

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Journal: A C S Catalysis
Volume: 5
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BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 10.3 SJR 4.299 SNIP 2.071
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 4.039 SNIP 2.134 CiteScore 9.88
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 3.641 SNIP 2.022 CiteScore 8.74
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 3.271 SNIP 1.859 CiteScore 7.41
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Scopus rating (2012): SJR 2.684 SNIP 1.61 CiteScore 5.19
ISI indexed (2012): ISI indexed no
Web of Science (2012): Indexed yes
ISI indexed (2011): ISI indexed no
Original language: English
SCR, Fast SCR, Rate-determining, Step, Mechanism, Cu-CHA, NO oxidation, EPR, EXAFS, FTIR, XANES, DFT
Electronic versions:
A_consistent_reaction_scheme.pdf
DOIs:
10.1021/cs501673g
Publication: Research - peer-review › Journal article – Annual report year: 2015

Adsorption of Cationic Peptides to Solid Surfaces of Glass and Plastic
Cationic membrane-active peptides have been studied for years in the hope of developing them into novel types of therapeutics. In this article, we investigate an effect that might have significant experimental implications for investigators who wish to study these peptides, namely, that the peptides adsorb to solid surfaces of glass and plastic. Specifically, we use analytical HPLC to systematically quantify the adsorption of the three cationic membraneactive peptides mastoparan X, melittin, and magainin 2 to the walls of commonly used glass and plastic sample containers. Our results show that, at typical experimental peptide concentrations, 90% or more of the peptides might be lost from solution due to rapid
adsorption to the walls of the sample containers. Thus, our results emphasize that investigators should always keep these adsorption effects in mind when designing and interpreting experiments on cationic membrane-active peptides. We conclude the article by discussing different strategies for reducing the experimental impact of these adsorption effects.

**General information**

State: Published

Organisations: Department of Micro- and Nanotechnology, Colloids and Biological Interfaces, Center for Nanomedicine and Theranostics, Department of Chemistry, Physical and Biophysical Chemistry

Authors: Kristensen, K. (Intern), Henriksen, J. R. (Intern), Andresen, T. L. (Intern)

Number of pages: 17

Publication date: 2015

Main Research Area: Technical/natural sciences

**Publication information**

Journal: *P L o S One*

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ISSN (Print): 1932-6203

Ratings:

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- Web of Science (2017): Indexed yes
- BFI (2016): BFI-level 1
- Web of Science (2016): Indexed yes
- BFI (2015): BFI-level 1
- Web of Science (2015): Indexed yes
- Scopus rating (2016): CiteScore 3.11 SJR 1.201 SNIP 1.092
- Web of Science (2016): Indexed yes
- BFI (2014): BFI-level 1
- Scopus rating (2014): SJR 1.545 SNIP 1.141 CiteScore 3.54
- Web of Science (2014): Indexed yes
- BFI (2013): BFI-level 1
- Scopus rating (2013): SJR 1.74 SNIP 1.147 CiteScore 3.94
- ISI indexed (2013): ISI indexed yes
- Web of Science (2013): Indexed yes
- BFI (2012): BFI-level 1
- Scopus rating (2012): SJR 1.945 SNIP 1.142 CiteScore 4.15
- ISI indexed (2012): ISI indexed yes
- Web of Science (2012): Indexed yes
- BFI (2011): BFI-level 1
- Scopus rating (2011): SJR 2.369 SNIP 1.23 CiteScore 4.58
- ISI indexed (2011): ISI indexed no
- Web of Science (2011): Indexed yes
- BFI (2010): BFI-level 1
- Scopus rating (2010): SJR 2.631 SNIP 1.161
- Web of Science (2010): Indexed yes
- BFI (2009): BFI-level 1
- Scopus rating (2009): SJR 2.473 SNIP 0.985
- Web of Science (2009): Indexed yes
- BFI (2008): BFI-level 1
- Scopus rating (2008): SJR 2.323 SNIP 0.96
- Web of Science (2008): Indexed yes
- Scopus rating (2007): SJR 1.289 SNIP 0.525
- Web of Science (2006): Indexed yes

Original language: English

Electronic versions:
Adsorption of Cationic Peptides.pdf

DOIs:
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Publication: Research - peer-review › Journal article – Annual report year: 2015

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

A Four-Component Reaction for the Synthesis of Dioxadiazaborocines

A four-component reaction for the synthesis of heterocyclic boronates is reported. Readily available hydrazides, α-hydroxy aldehydes, and two orthogonally reactive boronic acids are combined in a single step to give structurally distinct bicyclic boronates, termed dioxadiazaborocines (DODA borocines). In this remarkable process, one boronic acid reacts as a carbon nucleophile and the other as a boron electrophile to provide enantio- and diastereomerically pure heterocyclic boronates with multiple stereocenters in high yields.

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry
Authors: Flagstad, T. (Intern), Petersen, M. T. (Intern), Nielsen, T. E. (Intern)
Number of pages: 3
Pages: 8395-8397
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Volume: 54
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Web of Science (2018): Indexed yes
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
A Four‐Component Reaction for the Synthesis of Dioxadiazaborocines

A four‐component reaction for the synthesis of heterocyclic boronates is reported. Readily available hydrazides, α‐hydroxy aldehydes, and two orthogonally reactive boronic acids are combined in a single step to give structurally distinct bicyclic boronates, termed dioxadiazaborocines (DODA borocines). In this remarkable process, one boronic acid reacts as a carbon nucleophile and the other as a boron electrophile to provide enantio‐ and diastereomerically pure heterocyclic boronates with multiple stereocenters in high yields.

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry
Authors: Flagstad, T. (Intern), Petersen, M. T. (Intern), Nielsen, T. E. (Intern)
Number of pages: 3
A Higgs at 125.1 GeV and baryon mass spectra derived from a Common U(3) Lie group framework

Baryons are described by a Hamiltonian on an intrinsic U(3) Lie group configuration space with electroweak degrees of freedom originating in specific Bloch wave factors. By opening the Bloch degrees of freedom pairwise via a U(2) Higgs mechanism, the strong and electroweak energy scales become related to yield the Higgs mass 125.085±0.017 GeV and the usual gauge boson masses. From the same Hamiltonian we derive both the relative neutron to proton mass ratio and the N and Delta mass spectra. All compare rather well with the experimental values. We predict neutral flavour baryon singlets to be sought for in negative pions scattering on protons or in photoproduction on neutrons and in invariant mass like Σ+c(2455)D− from various decays above the open charm threshold, e.g. at 4499, 4652 and 4723 MeV. The fundamental predictions are based on just one length scale and the fine structure coupling. The interpretation is to consider baryons as entire entities kinematically excited from laboratory space by three impact momentum generators, three rotation generators and three Runge-Lenz generators to internalize as nine degrees of freedom covering colour, spin and flavour. Quark and gluon fields come about when the intrinsic structure is projected back into laboratory space depending on which exterior derivative one is taking. With such derivatives on the measure-scaled wavefunction, we derived approximate parton distribution functions for the u and d valence quarks of the proton that compare well with established experimental analysis.

General information
State: Published
Organisations: Department of Physics, Department of Chemistry
Authors: Trinhammer, O. (Intern), Bohr, H. (Intern), Jensen, M. O. S. (Intern)
Number of pages: 8
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: PoS - Proceedings of Science
Volume: 22-29
Article number: 097
ISSN (Print): 1824-8039
Ratings:
ISI indexed (2013): ISI indexed no
ISI indexed (2012): ISI indexed no
ISI indexed (2011): ISI indexed no
Original language: English
Electronic versions:
A_Higgs_at_125.1_GeV_and_baryon_mass_spectra_derived_from_a_Common_U_3_Lie_group_framework.pdf

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Source-ID: 2346427554
Publication: Research - peer-review › Conference article – Annual report year: 2016

A hydrogel based nanosensor with an unprecedented broad sensitivity range for pH measurements in cellular compartments

Optical pH nanosensors have been applied for monitoring intracellular pH in real-time for about two decades. However, the pH sensitivity range of most nanosensors is too narrow, and measurements that are on the borderline of this range may not be correct. Furthermore, ratiometric measurements of acidic intracellular pH (pH < 4) in living cells are still challenging due to the lack of suitable nanosensors. In this paper we successfully developed a multiple sensor, a fluorophore based nanosensor, with an unprecedented broad measurement range from pH 1.4 to 7.0. In this nanosensor, three pH-sensitive fluorophores (difluoro-Oregon Green, Oregon Green 488, and fluorescein) and one pH-insensitive fluorophore (Alexa 568) were covalently incorporated into a nanoparticle hydrogel matrix. With this broad range quadruple-
labelled nanosensor all physiological relevant pH levels in living cells can be measured without being too close to the limits of its pH-range. The nanosensor exhibits no susceptibility to interference by other intracellular ions at physiological concentrations. Due to its positive surface charge it is spontaneously internalized by HeLa cells and localizes to the lysosomes where the mean pH was measured at 4.6. This quadruple-labelled nanosensor performs accurate measurements of fluctuations of lysosomal pH in both directions, which was shown by treatment with the V-ATPase inhibitor bafilomycin A1 or its substrate ATP in HeLa cells. These measurements indicate that this novel quadruple-labelled nanosensor is a promising new tool for measuring the pH of acidic compartments in living cells.

General information
State: Published
Organisations: Department of Micro- and Nanotechnology, Colloids and Biological Interfaces, Department of Chemistry, Physical and Biophysical Chemistry, Organic Chemistry, Technical University of Denmark, Shanghai Jiao Tong University
Authors: Zhang, M. (Ekstern), Søndergaard, R. V. (Intern), Ek, P. K. (Intern), Henriksen, J. R. (Intern), Cui, D. (Ekstern), Hammershøj, P. (Intern), Clausen, M. H. (Intern), Andresen, T. L. (Intern)
Number of pages: 8
Pages: 7246-7253
Publication date: 2015
Main Research Area: Technical/natural sciences

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Journal: Analyst
Volume: 140
ISSN (Print): 0003-2654
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BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.92
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 4.07
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 4.1
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): CiteScore 4.11
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): CiteScore 3.88
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): CiteScore 4.16
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Web of Science (2006): Indexed yes
Web of Science (2005): Indexed yes
Web of Science (2002): Indexed yes
Web of Science (2001): Indexed yes
Allosteric small-molecule kinase inhibitors
Small-molecule kinase inhibitors are invaluable targeted therapeutics for the treatment of various human diseases, especially cancers. While the majority of approved and developed preclinical small-molecule inhibitors are characterized as type I or type II inhibitors that target the ATP-binding pocket of kinases, the remarkable sequential and structural similarity among ATP pockets renders the selective inhibition of kinases a daunting challenge. Therefore, targeting allosteric pockets of kinases outside the highly conserved ATP pocket has been proposed as a promising alternative to overcome current barriers of kinase inhibitors, including poor selectivity and emergence of drug resistance. In spite of the small number of identified allosteric inhibitors in comparison with that of inhibitors targeting the ATP pocket, encouraging results, such as the FDA-approval of the first small-molecule allosteric inhibitor trametinib in 2013, the progress of more than 10 other allosteric inhibitors in clinical trials, and the emergence of a pipeline of highly selective and potent preclinical molecules, have been reported in the past decade. In this article, we present the current knowledge on allosteric inhibition in terms of conception, classification, potential advantages, and summarized debatable topics in the field. Recent progress and allosteric inhibitors that were identified in the past three years are highlighted in this paper.
A study is presented on how well possible drug-molecules can be predicted with respect to their function and binding to a selection of G protein-coupled receptors by the use of artificial neural networks. The ligands investigated in this study are chosen to be corresponding to the G protein-coupled receptors mu-opioid, serotonin 2B (5-HT2B) and metabotropic glutamate D5. They are selected due to the availability of pharmacological drug-molecule binding data for these receptors. Feedback and deep belief artificial neural network architectures (NNs) were chosen to perform the task of aiding drug-design. This is done by training on structural features, selected using a "minimum redundancy, maximum relevance"-test, and testing for successful prediction of categorized binding strength. An extensive comparison of the neural network performances was made in order to select the optimal architecture. Deep belief networks, trained with greedy learning algorithms, showed superior performance in prediction over the simple feedback NNs. The best networks obtained scores of more than 90 % accuracy in predicting the degree of binding drug molecules to the mentioned receptors and with a maximal Matthew's coefficient of 0.925. The performance of 8 category networks (8 output classes for binding strength) obtained a prediction accuracy of above 60 %. After training the networks, tests were done on how well the systems could be used as an aid in designing candidate drug molecules. Specifically, it was shown how a selection of chemical characteristics could give the lowest observed IC50 values, meaning largest bio-effect pr. nM substance, around 0.03-0.06 nM. These ligand characteristics could be total number of atoms, their types etc. In conclusion, deep belief networks trained on drug-molecule structures were demonstrated as powerful computational tools, able to aid in drug-design in a fast and cheap fashion, compared to conventional pharmacological techniques.
We report a facile and low-cost approach for the preparation of all-in-one supercapacitor electrodes using copper foam (CuF) integrated three-dimensional (3D) reduced graphene oxide (rGO) networks. The binderfree 3DrGO@CuF electrodes are capable of delivering high specific capacitance approaching the theoretical capacitance of graphene and exhibiting high charge–discharge cycling stability.
Architecture and Applications of Functional Three-Dimensional Graphene Networks

As the first atomic-thick two-dimensional crystalline material, graphene has continuously created a wonder land in materials science within the past decade. A number of methods have been developed for preparation and functionalization of single-layered graphene nanosheets (GNS), which are essential building blocks for the bottom-up architecture of various graphene-based nanomaterials. The assembly of functionalized GNS into three-dimensional (3D) porous graphenennetworks represents a novel approach. Resulting 3D porous graphene materials possess unique physicochemical properties such as large surface areas, good conductivity and mechanical strength, high thermal stability and desirable flexibility, which altogether makes this new type of porous materials highly attractive for a wide range of applications. In this chapter, we will cover some crucial aspects of porous graphene networked materials based on the accomplishments recently reported. This chapter will include: (1) a brief introduction to graphene and its nanocomposites, (2) the major methods to assemble 3D porous graphenennetworks, (3) structural characteristics of 3D porous graphene, (4) some typical examples of their applications in sensors and energy devices, and (5) conclusions, remaining challenges and outlooks.

General information
State: Published
Organisations: Department of Chemistry, NanoChemistry
Authors: Dey, R. S. (Intern), Chi, Q. (Intern)
Number of pages: 33
Pages: 67-99
Publication date: 2015

Host publication information
Title of host publication: Graphene Materials : Fundamentals and Emerging Applications
Publisher: Scrivener Publishing
Editors: Tiwar, A., Syväjärvi, M.
ISBN (Print): 9781118998373
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Chapter: 3

Series: Advanced Materials Series
Main Research Area: Technical/natural sciences
Graphene, 3D porous graphene, Energy devices, Supercapacitors, Electrochemistry
DOIs: 10.1002/9781119131816.ch3
Publication: Research › Book chapter – Annual report year: 2015

A recycling pathway for cyanogenic glycosides evidenced by the comparative metabolic profiling in three cyanogenic plant species

Cyanogenic glycosides are phytoanticipins involved in plant defence against herbivores by virtue of their ability to release toxic HCN upon tissue disruption. In addition, endogenous turnover of cyanogenic glycosides without the liberation of HCN may offer plants an important source of reduced nitrogen at specific developmental stages. To investigate the presence of putative turnover products of cyanogenic glycosides, comparative metabolic profiling using LC-MS/MS and HR-MS complemented by ion-mobility mass spectrometry was carried out in three cyanogenic plant species: cassava, almond and sorghum. In total, the endogenous formation of 36 different chemical structures related to the cyanogenic glucosides linamarin, lotaustralin, prunasin, amygdalin and dhurrin was discovered, including di- and triglycosides derived from these compounds. The relative abundance of the compounds was assessed in different tissues and developmental stages. Based on results common to the three phylogenetically unrelated species, a potential recycling endogenous turnover pathway for cyanogenic glycosides is described in which reduced nitrogen and carbon are recovered for primary metabolism without the liberation of free HCN. Glycosides of amides, carboxylic acids and “anitriles” derived from cyanogenic glycosides appear as common intermediates in this pathway and may also have individual functions in the plant. The recycling of cyanogenic glycosides and the biological significance of the presence of the turnover products in cyanogenic plants open entirely new insights into the multiplicity of biological roles cyanogenic glycosides may play in plants.

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry, University of Copenhagen, University of Manchester
Authors: Pičmanová, M. (Ekstern), Neilson, E. H. (Forskerdatabase), Motawia, M. S. (Ekstern), Olsen, C. E. (Ekstern), Agerbirk, N. (Forskerdatabase), Gray, C. (Ekstern), Flitsch, S. (Ekstern), Meier, S. (Intern), Silvestro, D. (Ekstern), Jørgensen, K. (Forskerdatabase), Sánchez-Pérez, R. (Forskerdatabase), Møller, B. L. (Ekstern), Bjarnholt, N. (Ekstern)
Number of pages: 15
Pages: 375-389
Publication date: 2015
Main Research Area: Technical/natural sciences
Assembling Cysteine Monolayers on Low-Index Gold Surfaces

General information
State: Published
Organisations: Department of Chemistry, NanoChemistry, Organic Chemistry, Technical University of Denmark, Kazan National Research Technological University, Xiamen University
Authors: Engelbrekt, C. (Intern), Nazmutdinov, R. R. (Ekstern), Yan, J. (Ekstern), Zinkicheva, T. (Ekstern), Mao, B. (Ekstern), Ulstrup, J. (Intern), Zhang, J. (Intern)
Number of pages: 1
Publication date: 2015
Event: Abstract from The 8th International Workshop on Scanning Electrochemical Microscopy, Xiamen, China.
Main Research Area: Technical/natural sciences
Cysteine monolayers, Gold, Scanning tunneling microscopy, Voltammetry, DFT
Electronic versions:
Assembling_Cysteine_Monolayers_on_Low_Index_Gold_Surfaces.pdf
Source: PublicationPreSubmission
Source-ID: 118113302
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2015

Azido-RGO as a universal platform for RGO based sensors

General information
State: Published
Organisations: Department of Chemistry, NanoChemistry, Organic Chemistry
Authors: Olsen, G. (Intern), Ulstrup, J. (Intern), Chi, Q. (Intern)
Number of pages: 1
Publication date: 2015
Main Research Area: Technical/natural sciences
Electronic versions:
Azido_RGO_as_a_universal_platform_for_RGO_based_sensors.pdf
Source: PublicationPreSubmission
Source-ID: 118201904
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2015

Bacillus halodurans Strain C125 Encodes and Synthesizes Enzymes from Both Known Pathways To Form dUMP Directly from Cytosine Deoxyribonucleotides

Analysis of the genome of Bacillus halodurans strain C125 indicated that two pathways leading from a cytosine deoxyribonucleotide to dUMP, used for dTMP synthesis, were encoded by the genome of the bacterium. The genes that were responsible, the comEB gene and the dcdB gene, encoding dCMP deaminase and the bifunctional dCTP deaminase:dUTPase (DCD:DUT), respectively, were both shown to be expressed in B. halodurans, and both genes were subject to repression by the nucleosides thymidine and deoxycytidine. The latter nucleoside presumably exerts its repression after deamination by cytidine deaminase. Both comEB and dcdB were cloned, overexpressed in Escherichia coli, and purified to homogeneity. Both enzymes were active and displayed the expected regulatory properties: activation by dCTP for dCMP deaminase and dTTP inhibition for both enzymes. Structurally, the B. halodurans enzyme resembled the Mycobacterium tuberculosis enzyme the most. An investigation of sequenced genomes from other species of the genus Bacillus revealed that not only the genome of B. halodurans but also the genomes of Bacillus pseudofirmus, Bacillus thuringiensis, Bacillus hemocellulosilyticus, Bacillus marmarensis, Bacillus cereus, and Bacillus megaterium encode both the dCMP deaminase and the DCD:DUT enzymes. In addition, eight dcdb homologs from Bacillus species within the genus for which the whole genome has not yet been sequenced were registered in the NCBI Entrez database.

General information
State: Published
Organisations: Department of Chemistry, Department of Systems Biology, X-ray Crystallography, Metabolic Signaling and Regulation, Technical University of Denmark, University of Copenhagen
Authors: Oehlenschlæger, C. B. (Ekstern), Levgreen, M. N. (Intern), Reinauer, E. (Intern), Lehtinen, E. (Ekstern), Pind, M. L. (Ekstern), Harris, P. (Intern), Martinussen, J. (Intern), Willemoës, M. (Ekstern)
Bridging the Gap

Bridging the Gap (BtG) is a 2-year project funded by The Danish Industry Foundation. The goal of Bridging the Gap has been to create a new innovation model which will increase the rate at which Danish universities can spinout new technology ventures.

General information
State: Published
Organisations: Department of Chemistry, Department of Photonics Engineering, Department of Management Engineering, Technology and Innovation Management, Scientifica
Authors: Kramer Overgaard, M. (Intern), Broeng, J. (Intern), Jensen, M. L. (Intern), Murdock, K. (Intern), Schmidt, I. J. (Intern)
Number of pages: 13
Publication date: 2015

Publication information
Publisher: DTU Fotonik
Electronic versions:
ReportBtG_dec15web.pdf
Links:
http://www.bridgingthegap.dk

Bibliographical note
Main Research Area: Technical/natural sciences
Source: PublicationPreSubmission
Source-ID: 118885667
Publication: Research › Working paper – Annual report year: 2015

Bridging the gap from research-to-high-technology ventures with experienced entrepreneurs

The paper outlines an initiative undertaken to increase the number of spin-outs from a research university. The Bridging the Gap (BtG) model takes a systematic approach to identify and match experienced external entrepreneurs at a very early stage in the technological development process with university researchers to improve the technology spin-out process. The experiences, market insight and network connections of experienced entrepreneurs when combine with technical knowledge and capabilities of the researchers create a strong resource base for start-ups. This strong resource base can shorten the actual time taken to spin-out a technology and also increase the prospects for the emerging start-ups to achieve sustainable growth. The empirical evidence to support the model comes from two research departments at the Technical University of Denmark.

General information
State: Published
Organisations: Department of Chemistry, Department of Management Engineering, Technology and Innovation Management, Department of Photonics Engineering
Authors: Kramer Overgaard, M. (Intern), Murdock, K. (Intern), Jensen, M. L. (Intern), Broeng, J. (Intern)
Number of pages: 14
Publication date: 2015

Host publication information
Title of host publication: Proceedings of The XXVI ISPIM Conference 2015
Case report: a novel KERA mutation associated with cornea plana and its predicted effect on protein function

Background: Cornea plana (CNA) is a hereditary congenital abnormality of the cornea characterized by reduced corneal curvature, extreme hypermetropia, corneal clouding and hazy corneal limbus. The recessive form, CNA2, is associated with homozygous or compound heterozygous mutations of the keratocan gene (KERA) on chromosome 12q22. To date, only nine different disease-associated KERA mutations, including four missense mutations, have been described.

Case presentation: In this report, we present clinical data from a Turkish family with autosomal recessive cornea plana. In some of the affected individuals, hypotrichosis was found. KERA was screened for mutations using Sanger sequencing. We detected a novel KERA variant, p.(Ile225Thr), that segregates with the disease in the homozygous form. The three-dimensional structure of keratocan protein was modelled, and we showed that this missense variation is predicted to destabilize the structure of keratocan, leading to the classical ocular phenotype in the affected individuals. All the four known missense mutations, including the variation found in this family, affect the conserved residues of the leucine rich repeat domain of keratocan. These mutations are predicted to result in destabilization of the protein. Conclusion: We present the 10th pathogenic KERA mutation identified so far. Protein modelling is a useful tool in predicting the effect of missense mutations. This case underline the importance of the leucin rich repeat domain for the protein function, and this knowledge will ease the interpretation of future findings of mutations in these areas in other families with cornea plana.
Catalytic Alkylation of 2-Methylfuran with Formalin Using Supported Acidic Ionic Liquids

Biphasic alkylation of 2-methylfuran (2-MF) with formalin was carried out with a series of SBA-15 supported acidic ionic liquid catalysts (acidic SILCs) under mild reaction conditions. Acidic SILC with sulfonic acid groups (SO₃H) and long alkyl chains was observed to have higher catalytic activity than commercial sulfonic acid resin catalysts for the alkylation reaction in terms of TONs/TOFs as well as selectivity (90%) toward the C11 oxygenate bis(5-methylfuran-2-yl)methane (BMFM). The reaction product was easily separated by addition of the nonpolar solvent n-heptane and additional water to form a biphasic system. The reactivity of other biomass-based substrates such as 3,4-dimethoxybenzaldehyde, furfural, glycolaldehyde, and glyceraldehyde was also investigated over acidic SILCs, and excellent yields of about 80% or higher were obtained of the corresponding condensed products (except from glyceraldehyde). Easy catalyst recovery from the aqueous phase after extraction of BMFM with n-heptane and reusability for at least five consecutive reaction runs without significant loss of catalyst activity was further exemplified for a selected catalyst.

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry, Technical University of Denmark, Guizhou University
Authors: Li, H. (Ekstern), Shunmugavel, S. (Intern), Yang, S. (Ekstern), Riisager, A. (Intern)
Number of pages: 7
Pages: 374-3280
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: A C S Sustainable Chemistry & Engineering
Volume: 3
Issue number: 12
ISSN (Print): 2168-0485
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
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

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Title of host publication: Book of Abstracts. DTU's Sustain Conference 2015
Place of publication: Lyngby
Publisher: Technical University of Denmark (DTU)
Article number: R-20
Main Research Area: Technical/natural sciences
Conference: DTU Sustain Conference 2015, Lyngby, Denmark, 17/12/2015 - 17/12/2015
Electronic versions:
R20_DTU_Sustain_2015.pdf

Bibliographical note
Poster presentation
Publication: Research - peer-review › Conference abstract in proceedings – 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)
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
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

Characterization of cellulose fibers by powder diffraction

General information
State: Published
Organisations: Department of Chemistry, X-ray Crystallography, Organic Chemistry, Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering
Authors: Ståhl, K. (Intern), Frankær, C. G. (Intern), Guldbech, T. K. (Intern), Thygesen, A. (Intern)
Number of pages: 1
Publication date: 2015
Event: Abstract from The 29th European Crystallographic Meeting, Rovinj, Croatia.
Main Research Area: Technical/natural sciences
Electronic versions:
Characterization_of_cellulose_fibers_by_powder_diffraction.pdf
Source: PublicationPreSubmission
Source-ID: 116663812
Publication: Research - peer-review › Poster – Annual report year: 2015

Characterization of four new antifungal yanuthones from Aspergillus niger
Four new yanuthone analogs (1–4) were isolated from the filamentous fungus Aspergillus niger. The structures of the new compounds were elucidated on the basis of UHPLC-DAD-HRMS data and one-dimensional and two-dimensional NMR spectroscopy. Labeling studies with 13C8-6-methylsalicylic acid identified three class I yanuthones originating from the polyketide 6-methylsalicylic acid (yanuthone K, L and M (1–3)) and a class II yanuthone, which was named yanuthone X2 (4). The four new compounds were tested toward the pathogenic yeast Candida albicans and all displayed antifungal activity. Yanuthone X2 represents the first example of a bioactive class II yanuthone, demonstrating the pharmaceutical potential of this class.

General information
State: Published
Organisations: Department of Systems Biology, Department of Chemistry, Organic Chemistry, Fungal Physiology and Biotechnology, Metabolomics Platform, Eucaryotic Molecular Cell Biology, Fermentation Platform
Number of pages: 5
Pages: 201-205
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: The Journal of Antibiotics
Volume: 68
ISSN (Print): 0021-8820
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
Charge regulation and energy dissipation while compressing and sliding a cross-linked chitosan hydrogel layer

Interactions between a silica surface and a surface coated with a grafted cross-linked hydrogel made from chitosan/PAA multilayers are investigated, utilizing colloidal probe atomic force microscopy. Attractive double-layer forces are found to dominate the long-range interaction over a broad range of pH and ionic strength conditions. The deduced potential at the hydrogel/aqueous interface is found to be very low. This situation is maintained in the whole pH-range investigated, even though the degree of protonation of chitosan changes significantly. This demonstrates that pH-variations change the concentration of counterions within the hydrogel to keep the interior close to uncharged, which is similar to what has been observed for polyelectrolyte brushes. Changes in pH and ionic strength affect the adhesion force and the friction force between the silica surface and the hydrogel layer, but not the friction coefficient. This suggests that the main energy dissipation mechanism arises from processes occurring within the hydrogel layer, rather than at the silica/hydrogel interface, and we suggest that it is related to stretching of polymer chains between the cross-linking points. We also find that an increased cross-linking density, from 40% to 100%, in the hydrogel reduces the friction coefficient.
Chemistry of the active metal center in the selective catalytic reduction of NO by NH₃

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry
Authors: Mossin, S. (Intern)
Number of pages: 2
Publication date: 2015
Main Research Area: Technical/natural sciences
Electronic versions:
EuropaCatLongAbstract_Mossin.pdf

Chemoselective Oxidation of Bio-Glycerol with Nano-Sized Metal Catalysts
Glycerol, a major co-product in the process of biodiesel production, is a promising precursor to a variety of high value fine chemicals such as glyceric acid, dihydroxyacetone, lactic acid and tartronic acid via the corresponding chemoselective oxidation reactions. One of the prospective routes to selectively oxidize glycerol and yield products with good selectivity is the use of nano-sized metal particles as heterogeneous catalysts. In this short review, recent developments in chemoselective oxidation of glycerol to specific products over nano-sized metal catalysts are described. Attention is drawn to various reaction parameters such as the type of the support, the size of the metal particles, and the acid/base properties of the reaction medium which were illustrated to largely influence the activity of the nanocatalyst and selectivity to the target product. - See more at: http://www.eurekaselect.com/125706/article#sthash.gb2nV9Cq.dpuf

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Guizhou University, Technical University of Denmark
Authors: Li, H. (Ekstern), Kotni, R. (Ekstern), Zhang, Q. (Ekstern), Shunmugavel, S. (Intern), Yang, S. (Ekstern)
Number of pages: 16
Pages: 162-177
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Mini - Reviews in Organic Chemistry
Volume: 12
Issue number: 2
ISSN (Print): 1570-193X
Ratings:
Web of Science (2018): Indexed yes
CO2 adsorbers for upgrading of bio-gas to methane

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry
Authors: Schill, L. (Intern), Riisager, A. (Intern), Fehrmann, R. (Intern)
Number of pages: 1
Publication date: 2015

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Title of host publication: Book of Abstracts. DTU's Sustain Conference 2015
Place of publication: Lyngby
Publisher: Technical University of Denmark (DTU)
Article number: E-31
Main Research Area: Technical/natural sciences
Conference: DTU Sustain Conference 2015, Lyngby, Denmark, 17/12/2015 - 17/12/2015
Electronic versions:
E31_DTU_Sustain_2015.pdf

Bibliographical note
Poster presentation
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2015

Coherent Control of Photofragment Distributions Using Laser Phase Modulation in the Weak-Field Limit
The possibility of quantum interference control of the final state distributions of photodissociation fragments by means of pure phase modulation of the pump laser pulse in the weak-field regime is demonstrated theoretically for the first time. The specific application involves realistic wave packet calculations of the transient vibrational populations of the Br2(B, vf) fragment produced upon predissociation of the Ne-Br2(B) complex, which is excited to a superposition of resonance states using pulses with different linear chirps. Transient phase effects on the fragment populations are found to persist for long times (about 200 ps) after the pulse is over due to interference between overlapping resonances in Ne-Br2(B).

General information
State: Published
Organisations: Department of Chemistry, Physical and Biophysical Chemistry, Consejo Superior de Investigaciones Científicas
Authors: Garcia-Vela, A. (Ekstern), Henriksen, N. E. (Intern)
Number of pages: 6
Pages: 824-829
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Building on recent advances in the rotational excitation of molecules, we show how the effect of rotation-vibration coupling can be switched on in a controlled manner and how this coupling unfolds in real time after a pure rotational excitation. We present the first examination of the vibrational motions which can be induced via the rotation-vibration coupling after a pulsed rotational excitation. A time-dependent quantum wave packet calculation for the HF molecule shows how a slow (compared to the vibrational period) rotational excitation leads to a smooth increase in the average bond length whereas a
fast rotational excitation leads to a non-stationary vibrational motion. As a result, under field-free postpulse conditions, either a stretched stationary bond or a vibrating bond can be created due to the coupling between the rotational and vibrational degrees of freedom. The latter corresponds to a laser-induced breakdown of the adiabatic approximation for rotation-vibration coupling.
Copper oxide as efficient catalyst for oxidative dehydrogenation of alcohols with air

The oxidative dehydrogenation of alcohols to carbonyl compounds was studied using CuO nanoparticle catalysts prepared by solution synthesis in buffered media. CuO nanoparticles synthesized in N-cyclohexyl-3-aminopropanesulfonic acid...
buffer showed high catalytic activity for the oxidation of benzylic, alicyclic and unsaturated alcohols to their corresponding carbonyl compounds with excellent selectivities. The observed trend in activity for conversion of substituted alcohols suggested a β-H elimination step to be involved, thus enabling a possible reaction mechanism for oxidative dehydrogenation of benzyl alcohols to be proposed. The use of CuO as an inexpensive and efficient heterogeneous catalyst under aerobic conditions provides a new noble metal-free and green reaction protocol for carbonyl compound synthesis.

**General information**
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, NanoChemistry
Authors: Poreddy, R. (Intern), Engelbrekt, C. (Intern), Riisager, A. (Intern)
Number of pages: 11
Pages: 2467-2477
Publication date: 2015
Main Research Area: Technical/natural sciences

**Publication information**
Journal: Catalysis Science & Technology
Volume: 5
Issue number: 4
ISSN (Print): 2044-4753
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 5.64 SJR 1.795 SNIP 1.288
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.838 SNIP 1.319 CiteScore 5.46
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.897 SNIP 1.485 CiteScore 5.44
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.776 SNIP 1.343 CiteScore 4.89
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Scopus rating (2012): SJR 1.649 SNIP 1.013 CiteScore 3.7
ISI indexed (2012): ISI indexed no
ISI indexed (2011): ISI indexed no
Original language: English
Electronic versions: CuO_re_revised.pdf. Embargo ended: 10/02/2016
DOIs: 10.1039/c4cy01622j
Source: PublicationPreSubmission
Source-ID: 106096833
Publication: Research - peer-review › Journal article – Annual report year: 2015

**Cyclic N-acyliminium ions for the diversity-oriented synthesis of functionalized γ-lactams**

**General information**
State: Published
Organisations: Department of Chemistry, Organic Chemistry
Authors: Wu, P. (Intern), Nielsen, T. E. (Intern), Clausen, M. H. (Intern)
Number of pages: 1
Publication date: 2015
Event: Abstract from 250th American Chemical Society National Meeting & Exposition, Boston, United States.
Deactivation of solid catalysts in liquid media: the case of leaching of active sites in biomass conversion reactions

This review is aimed to be a brief tutorial covering the deactivation of solid catalysts in the liquid phase, with specific focus on leaching, which can be especially helpful to researchers not familiarized with catalytic processes in the liquid phase. Leaching refers to the loss of active species from the solid that are transferred into the liquid medium, causing eventually a deactivation of the catalyst. Intriguingly, not many published studies have dealt with leaching, since this is a specific phenomenon in the liquid phase and heterogeneous catalysis is mainly carried out in gaseous phase. However, as a consequence of the development of new processes for biorefineries, an increasing number of reactions deal with liquid media, and thus, the stability and reusability of a solid catalyst in this situation represent a huge challenge that requires specific attention. Leaching of active phases is particularly problematic because of its irreversibility and it can be one of the main causes of catalyst deactivation in liquid media, threatening the sustainability of the process. This tutorial review presents a survey of the main aspects concerning the deactivation due to leaching of active species from the solid catalyst such as mechanisms, detection methods, impact of these factors on global activity and finally, some procedures to try and minimize the leaching or to cope with it. A decision flowchart is presented to help in the study of catalyst stability and reusability. Interesting biomass conversion reactions have been chosen as examples to illustrate the importance of these aspects.

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Haldor Topsoe AS, CSIC
Authors: Sádaba, I. (Ekstern), Lopez Granados, M. (Ekstern), Riisager, A. (Intern), Taarning, E. (Ekstern)
Number of pages: 13
Pages: 4133-4145
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Journal: Green Chemistry
Volume: 17
Issue number: 8
ISSN (Print): 1463-9262
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 8.86 SJR 2.564 SNIP 2.019
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
Densities of the Binary Systems n-Hexane + n-Decane and n-Hexane + n-Hexadecane up to 60 MPa and 463 K

The densities of the binary systems n-hexane + n-decane and n-hexane + n-hexadecane have been measured up to 60 MPa using a vibrating tube densimeter. The measurements covered the whole composition range; for the first system they were performed from (278.15 to 463.15) K, while for the latter they were performed from (298.15 to 463.15) K because n-hexadecane is a solid at 278.15 K. The densities were correlated for every composition as a function of temperature and pressure using a modified Tammann-Tait equation with standard deviations lower than 8·10-4 g·cm-3. Isothermal compressibility values were calculated from the experimental density data. Moreover, the excess volumes were found to be negative for all of the studied mixtures, with absolute values less than or equal to 3.25 cm3·mol-1 for the n-hexane + n-decane system and 7.65 cm3·mol-1 for the n-hexane + n-hexadecane system. Various equations of state were used to model the measured density data.

**General information**

State: Published
Organisations: Department of Chemistry, CERE – Center for Energy Resources Engineering, Center for Energy Resources Engineering
Authors: Regueira, T. (Intern), Yan, W. (Intern), Stenby, E. H. (Intern)
Pages: 3631-3645
Publication date: 2015
Main Research Area: Technical/natural sciences
Detailed Characterization of a Nanosecond-Lived Excited State: X-ray and Theoretical Investigation of the Quintet State in Photoexcited [Fe(terpy)(2)][(2+)]

Theoretical predictions show that depending on the populations of the Fe 3d(xy), 3d(xz), and 3d(yz) orbitals two possible quintet states can exist for the high-spin state of the photoswitchable model system [Fe(terpy)(2)][(2+)]. The differences in the structure and molecular properties of these B-5(2) and E-5 quintets are very small and pose a substantial challenge for experiments to resolve them. Yet for a better understanding of the physics of this system, which can lead to the design of novel molecules with enhanced photoswitching performance, it is vital to determine which high-spin state is reached in the transitions that follow the light excitation. The quintet state can be prepared with a short laser pulse and can be studied with cutting-edge time-resolved X-ray techniques. Here we report on the application of an extended set of X-ray spectroscopy and scattering techniques applied to investigate the quintet state of [Fe(terpy)(2)][(2+) 80 ps after light excitation. High-quality X-ray absorption, nonresonant emission, and resonant emission spectra as well as X-ray diffuse scattering data clearly reflect the formation of the high-spin state of the [Fe(terpy)(2)][(2+) molecule; moreover, extended X-ray absorption fine structure spectroscopy resolves the Fe-ligand bond-length variations with unprecedented bond-length accuracy in time-resolved experiments. With ab initio calculations we determine why, in contrast to most related systems, one configurational mode is insufficient for the description of the low-spin (LS)-high-spin (HS) transition. We identify the electronic structure origin of the differences between the two possible quintet modes, and finally, we unambiguously identify the formed quintet state as 5E, in agreement with our theoretical expectations.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Risø National Laboratory for Sustainable Energy, Center for Atomic-scale Materials Design, Department of Chemistry, Physical and Biophysical Chemistry, Hungarian Academy of Sciences, Argonne National Laboratory, The Hamburg Centre for Ultrafast Imaging, European XFEL, European Synchrotron Radiation Facility
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BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.027 SNIP 1.448 CiteScore 5.08
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 2.134 SNIP 1.439 CiteScore 5.14
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.514 SNIP 1.46 CiteScore 4.98
Development of 3D-graphene for Biofuel Cells

General information
State: Published
Organisations: Department of Chemistry, NanoChemistry, Organic Chemistry
Authors: Wagner, M. (Intern), Ulstrup, J. (Intern), Zhang, J. (Intern)
Number of pages: 1
Publication date: 2015
Main Research Area: Technical/natural sciences
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Abstract for poster presentation
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Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2015

Development of brewing science in (and since) the late 19th century: molecular profiles of 110-130 year old beers

The 19th century witnessed many advances in scientific enzymology and microbiology that laid the foundations for modern biotechnological industries. In the current study, we analyze the content of original lager beer samples from the 1880s, 1890s and 1900s with emphasis on the carbohydrate content and composition. The historic samples include the oldest samples brewed with pure Saccharomyces carlsbergensis yeast strains. While no detailed record of beer pasteurization at the time is available, historic samples indicate a gradual improvement of bottled beer handling from the 1880s to the 1900s, with decreasing contamination by enzymatic and microbial activities over this time span. Samples are sufficiently
well preserved to allow comparisons to present-day references, thus yielding molecular signatures of the effects of 20th
century science on beer production. Opposite to rather stable carbohydrate profiles, some aldehydes reach up to 40-fold
higher levels in the historic samples as compared to present-day references.

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry, Carlsberg Laboratory
Authors: Walther, A. (Ekstern), Ravasio, D. (Ekstern), Qin, F. (Ekstern), Wendland, J. (Ekstern), Meier, S. (Intern)
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Web of Science (2018): Indexed yes
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Web of Science (2017): Indexed yes
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Scopus rating (2016): CiteScore 4.85 SJR 1.706 SNIP 2.091
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.597 SNIP 1.962 CiteScore 4.31
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.595 SNIP 2.027 CiteScore 3.92
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.548 SNIP 2.069 CiteScore 3.87
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.805 SNIP 2.357 CiteScore 3.98
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.909 SNIP 2.395 CiteScore 4.17
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.965 SNIP 2.261
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.776 SNIP 2.024
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.488 SNIP 1.703
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.467 SNIP 2.095
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.383 SNIP 1.848
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.017 SNIP 1.543
Development of the Molybdenum—Catalyzed Deoxydehydration of Polyols

General information
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Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2015

DFT Study of the Molybdenum-Catalyzed Deoxydehydration of Vicinal Diols.
The mechanism of the molybdenum-catalyzed deoxydehydration (DODH) of vicinal diols has been investigated using density functional theory. The proposed catalytic cycle involves condensation of the diol with an MoVI oxo complex, oxidative cleavage of the diol resulting in an MoV complex, and extrusion of the alkene. We have compared the proposed pathway with several alternatives, and the results have been corroborated by comparison with the molybdenum- catalyzed sulfoxide reduction recently published by Sanz et al. and with experimental observations for the DODH itself. Improved understanding of the mechanism should expedite future optimization of molybdenum-catalyzed biomass transformations.

General information
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Organisations: Department of Chemistry, Organic Chemistry
Authors: Lupp, D. (Intern), Christensen, N. J. (Intern), Dethlefsen, J. R. (Intern), Fristrup, P. (Intern)
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Publication information
Journal: Chemistry: A European Journal
Dimethylzinc-Initiated Radical Coupling of β-Bromostyrenes with Ethers and Amines

A new coupling reaction has been developed in which β-bromostyrenes react with ethers and tertiary amines to introduce the styryl group in the α-position. The transformation is mediated by Me₂Zn/O₂ with 10% MnCl₂ and is believed to proceed by a radical addition-elimination mechanism. The ether and the amine are employed as solvent and the coupling takes place through the most stable α radical for unsymmetrical substrates. The products are obtained in moderate to good yields as the pure E isomers. The coupling can be achieved with a range of smaller cyclic and acyclic ethers/amines as well as various substituted β-bromostyrenes.

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry
Authors: Sølvhøj, A. B. (Intern), Ahlburg, A. (Intern), Madsen, R. (Intern)
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Scopus rating (2015): SJR 2.416 SNIP 1.184 CiteScore 4.99
Web of Science (2015): Indexed yes
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Scopus rating (2014): SJR 2.487 SNIP 1.219 CiteScore 5.51
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Scopus rating (2013): SJR 2.604 SNIP 1.239 CiteScore 5.68
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Scopus rating (2012): SJR 2.884 SNIP 1.294 CiteScore 5.55
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 2.726 SNIP 1.336 CiteScore 5.46
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 2.527 SNIP 1.292
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.499 SNIP 1.365
We report a systematic analysis of conformational ensembles generated from multiseed molecular dynamics simulations of all 15 known genetic variants of Aβ42. We show that experimentally determined variant toxicities are largely explained by random coil content of the amyloid ensembles (correlation with smaller EC50 values; $R^2 = 0.54$, $p = 0.01$), and to some extent the helix character (more helix-character is less toxic, $R^2 = 0.32$, $p = 0.07$) and hydrophobic surface ($R^2 = 0.37$, $p = 0.04$). Our findings suggest that qualitative structural features of the amyloids, rather than the quantitative levels, are fundamentally related to neurodegeneration. The data provide molecular explanations for the high toxicity of E22 variants and for the protective features of the recently characterized A2T variant. The identified conformational features, for example, the local helix-coil-strand transitions of the C-terminals of the peptides, are of likely interest in the direct targeting of amyloids by rational drug design.
Discovery and optimization of peptide-based anti-cobratoxins

More than 5.5 million people per year are victims of snake envenomation, resulting in 125,000 deaths and 400,000 amputations worldwide. Antivenoms are still produced by animal immunization procedures, and they are associated with a high risk of severe adverse reactions. Alternatively, synthetic peptides may open the possibility for new therapies with better efficacy and safety. Here, we report the discovery and optimization of a synthetic peptide directed against α-cobratoxin (α-CTX), the most toxic component of Monocled cobra (Naja kaouthia).

DNA bases assembled on the Au(110)/electrolyte interface: A combined experimental and theoretical study

Among the low-index single-crystal gold surfaces, the Au(110) surface is the most active toward molecular adsorption and the one with fewest electrochemical adsorption data reported. Cyclic voltammetry (CV), electrochemically controlled scanning tunneling microscopy (EC-STM), and density functional theory (DFT) calculations have been employed in the present study to address the adsorption of the four nucleobases adenine (A), cytosine (C), guanine (G), and thymine (T), on the Au(110)-electrode surface. Au(110) undergoes reconstruction to the (1 × 3) surface in electrochemical environment, accompanied by a pair of strong voltammetry peaks in the double-layer region in acid solutions. Adsorption of the DNA bases gives featureless voltammograms with lower double-layer capacitance, suggesting that all the bases are chemisorbed on the Au(110) surface. Further investigation of the surface structures of the adlayers of the four DNA bases by EC-STM disclosed lifting of the Au(110) reconstruction, specific molecular packing in dense monolayers, and pH dependence of the A and G adsorption. DFT computations based on a cluster model for the Au(110) surface were performed to investigate the adsorption energy and geometry of the DNA bases in different adsorbate orientations. The optimized geometry is further used to compute models for STM images which are compared with the recorded STM images. This has provided insight into the physical nature of the adsorption. The specific orientations of A, C, G, and T on Au(110) and the nature of the physical adsorbate/surface interaction based on the combination of the experimental and theoretical studies are proposed, and differences from nucleobase adsorption on Au(111)-and Au(100)-electrode surfaces are discussed.
Dynamic behavior of impurities and native components in model LSM microelectrodes on YSZ

Strontium-doped lanthanum manganite is a widely used cathode material in solid oxide fuel cells. Segregation phenomena can have a critical impact on performance and durability, especially when they cause active interfaces to degrade. The segregation behavior in polarized and non-polarized strontium-doped lanthanum manganite ((La0.75Sr0.25)0.95MnO3) microelectrodes with a diameter of 100 μm and a thickness of ~500 nm on an yttria-stabilized zirconia electrolyte were analyzed post-mortem after ~200 h at temperatures up to 850 °C. Time-of-flight secondary ion mass spectrometry was used to study the dynamic behavior of the native components (La, Sr, Mn) and selected impurities (Si, K, Na) both laterally and in-depth. Manganese was found to be especially mobile and showed both segregation onto the electrolyte as a result of temperature and polarization and dissolution into the electrolyte below the microelectrodes. All native components showed a complex in-depth dynamic behavior, and a nanoscale in-depth analysis of the electrode-electrolyte interface revealed the formation of a well-defined lanthanum zirconate layer. The selected impurities segregated to the electrolyte and microelectrode surfaces and Na- and K-rich layers formed at different depths.
Effects of Coke Deposits on the Catalytic Performance of Large Zeolite H-ZSM-5 Crystals during Alcohol-to-Hydrocarbons Reactions as Investigated by a Combination of Optical Spectroscopy and Microscopy

The catalytic activity of large zeolite H-ZSM-5 crystals in methanol (MTO) and ethanol-to-olefins (ETO) conversions was investigated and, using operando UV/Vis measurements, the catalytic activity and deactivation was correlated with the formation of coke. These findings were related to in situ single crystal UV/Vis and confocal fluorescence micro-spectroscopy, allowing the observation of the spatiotemporal formation of intermediates and coke species during the MTO and ETO conversions. It was observed that rapid deactivation at elevated temperatures was due to the fast formation of aromatics at the periphery of the H-ZSM-5 crystals, which are transformed into more poly-aromatic coke species at the external surface, preventing the diffusion of reactants and products into and out of the H-ZSM-5 crystal. Furthermore, we were able to correlate the operando UV/Vis spectroscopy results observed during catalytic testing with the single crystal in situ results.
Effects of thionation and fluorination on cis-trans isomerization in tertiary amides: An investigation of N-alkylglycine (Peptoid) rotamers

Peptoids constitute a class of peptidomimetics with potential as protease resistant, biologically active ligands. To harness the full potential of such compounds, however, detailed predictive insight into their propensity to adopt well-defined secondary structures is highly desirable. In this work we present an investigation of the effects of thioamides and/or fluorides in peptoid monomer model systems using chemical synthesis, NMR spectroscopy, and X-ray crystallography. We
find that the steric environment surrounding the tertiary amide bonds is the key promoter of conformational preference, and X-ray crystallographic interrogation of our model systems did not suggest the presence of stabilizing $n \rightarrow \pi^*$ interactions unless the carbonyls were altered electronically by $\alpha$-halogenation or thioamide formation. In addition to the function as an investigative tool, these two types of modification may thus be utilized as stabilizers of secondary structure in future oligomer designs, such as the cis-amide-based polypeptoid helices that resemble the polyproline type-I helix.

**General information**

State: Published
Organisations: Department of Chemistry, Organic Chemistry, X-ray Crystallography, University of Copenhagen
Authors: Engel-Andreasen, J. (Intern), Wich, K. (Ekstern), Laursen, J. S. (Ekstern), Harris, P. (Intern), Olsen, C. A. (Intern)
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  - BFI (2016): BFI-level 2
  - Scopus rating (2016): CiteScore 4.59 SJR 1.976 SNIP 1.03
  - Web of Science (2016): Indexed yes
  - BFI (2015): BFI-level 2
  - Scopus rating (2015): SJR 2.018 SNIP 1.174 CiteScore 4.69
  - Web of Science (2015): Indexed yes
  - BFI (2014): BFI-level 2
  - Scopus rating (2014): SJR 2.003 SNIP 1.222 CiteScore 4.69
  - Web of Science (2014): Indexed yes
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  - Scopus rating (2013): SJR 2.078 SNIP 1.176 CiteScore 4.51
  - ISI indexed (2013): ISI indexed yes
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  - ISI indexed (2011): ISI indexed yes
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  - Scopus rating (2010): SJR 2.112 SNIP 1.173
  - BFI (2009): BFI-level 2
  - Scopus rating (2009): SJR 2.186 SNIP 1.254
  - Web of Science (2009): Indexed yes
  - BFI (2008): BFI-level 2
  - Scopus rating (2008): SJR 2.309 SNIP 1.208
  - Web of Science (2008): Indexed yes
  - Scopus rating (2007): SJR 2.37 SNIP 1.309
  - Web of Science (2007): Indexed yes
  - Scopus rating (2006): SJR 2.222 SNIP 1.31
Electroactive and Optoelectronically Active Graphene Nanofilms

As an atomic-scale-thick two-dimensional material, graphene has emerged as one of the most miracle materials and has generated intensive interest in physics, chemistry and even biology in the last decade [1, 2]. Nanoscale engineering and functionalization of graphene is a crucial step for many applications ranging from catalysis, electronic devices, sensors to advanced energy conversion and storage [3]. This talk highlights our recent studies on electroactive and optoelectronically active graphene ultrathin films for chemical sensors and energy technology. The presentation includes a general theme for functionalization of graphene nanosheets, followed by showing several case studies. Our systems cover redox-active nanoparticles, electroactive supramolecular ensembles and redox enzymes which are integrated with graphene nanosheets as building blocks for the construction of functional thin films or graphene papers.

Electrocatalysis of chemically synthesized noble metal nanoparticles on carbon electrodes

Noble metal nanoparticles (NPs), such as platinum (Pt) and palladium (Pd) NPs are promising catalysts for dioxygen reduction and oxidation of molecules such as formic acid and ethanol in fuel cells. Carbon nanomaterials are ideal supporting materials for electrochemical catalysts due to their good conductivity, chemical inertness and low cost. Improvement of catalytic efficiency and stability of the NPs is, however, essential for their wider applications in electrochemical energy conversion/storage. The activities of noble metal catalysts depend not only on their size, composition, and shapes but also on their interfacial interaction with the supporting electrodes. In this work we aim at chemical production of size and shape controlled, specifically 22 nm cubic Pd NPs, and further understanding of the Pd NPs as electrocatalysts at the nanometer scale using both scanning tunneling microscopy (STM) and atomic force microscopy (AFM) which have proved to be highly efficient techniques to map the in situ structures of selfassembled molecular monolayers at molecular or sub-molecular resolution. Electrocatalysis of the Pd NPs immobilized on atomically flat, highly oriented pyrolytic graphite (HOPG) will be investigated by electrochemical SPM. This study offers promise for development of new high-efficiency catalyst type with low-cost for fuel cell technology.
Electrochemically active dopamine functionalized graphene for sensor application

Electrochemical Single-Molecule Transistors with Optimized Gate Coupling

Electrochemically active dopamine functionalized graphene for sensor application

General information
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Organisations: Department of Chemistry, NanoChemistry, Organic Chemistry
Authors: Halder, A. (Intern), Ulstrup, J. (Intern), Chi, Q. (Intern)
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Main Research Area: Technical/natural sciences
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Source: PublicationPreSubmission
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Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2015

Electrochemical gating at the single molecule level of viologen molecular bridges in ionic liquids is examined. Contrary to previous data recorded in aqueous electrolytes, a clear and sharp peak in the single molecule conductance versus electrochemical potential data is obtained in ionic liquids. These data are rationalized in terms of a two-step electrochemical model for charge transport across the redox bridge. In this model the gate coupling in the ionic liquid is found to be fully effective with a modeled gate coupling parameter, $\xi$, of unity. This compares to a much lower gate coupling parameter of 0.2 for the equivalent aqueous gating system. This study shows that ionic liquids are far more effective media for gating the conductance of single molecules than either solid-state three-terminal platforms created using nanolithography, or aqueous media.

General information
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Organisations: Department of Chemistry, NanoChemistry, Universidad de Zaragoza, University of Liverpool, University of Western Australia, University of Reading
Authors: Osorio, H. M. (Ekstern), Catarelli, S. (Ekstern), Cea, P. (Ekstern), Gluyas, J. B. G. (Ekstern), Hartl, F. (Ekstern), Higgins, S. J. (Ekstern), Leary, E. (Ekstern), Low, P. J. (Ekstern), Martín, S. (Ekstern), Nichols, R. J. (Ekstern), Tory, J. (Ekstern), Ulstrup, J. (Intern), Vezzoli, A. (Ekstern), Milan, D. C. (Ekstern), Zeng, Q. (Ekstern)
Number of pages: 10
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Main Research Area: Technical/natural sciences

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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
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Environmental TEM study of the dynamic nanoscaled morphology of NiO/YSZ during reduction

The reduction of a metal oxide is often a critical preparation step for activating catalytic behaviour. This study addresses the reduction process of NiO in pure form and in a composite of NiO/yttria-stabilized zirconia (YSZ) in hydrogen relevant for solid oxide electrochemical cells by comparing results from environmental transmission electron microscopy (ETEM) with thermogravimetric analysis (TGA). The temperature dependent reduction profiles obtained from TGA confirm an inhibitive effect from YSZ on the NiO reduction. The ETEM images show the growth of Ni in decaying NiO and reveal the nanoscale morphological changes such as pore formation in NiO above 280°C and densification and collapse of the pore structures above 400°C. The accelerated Ni front in NiO illustrates the auto catalysis of the reaction. A rapid temperature ramping from room temperature to 780°C in hydrogen in 1 second resulted in immediate morphological changes at the nanoscale from dense NiO to dense Ni. The analysis suggests that the inhibitive effect of YSZ on the NiO reduction reaction is not due to a direct local interaction between YSZ and NiO, but instead due to gas and/or mass transport limitations.© 2014 Elsevier B.V. All rights reserved.

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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
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Scopus rating (2016): CiteScore 4.26 SJR 1.178 SNIP 1.311
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
Enzymatic degradation of lignin-carbohydrate complexes (LCCs): Model studies using a fungal glucuronoyl esterase from Cerrena unicolor

Lignin-carbohydrate complexes (LCCs) are believed to influence the recalcitrance of lignocellulosic plant material preventing optimal utilization of biomass in e.g. forestry, feed and biofuel applications. The recently emerged carbohydrate esterase (CE) 15 family of glucuronoyl esterases (GEs) has been proposed to degrade ester LCC bonds between glucuronic acids in xylans and lignin alcohols thereby potentially improving delignification of lignocellulosic biomass when applied in conjunction with other cellulases, hemicellulases and oxidoreductases. Herein, we report the synthesis of four new GE model substrates comprising α- and γ-arylalkyl esters representative of the lignin part of naturally occurring ester LCCs as well as the cloning and purification of a novel GE from Cerrena unicolor (CuGE). Together with a known GE from Schizophyllum commune (ScGE), CuGE was biochemically characterized by means of Michaelis–Menten kinetics with respect to substrate specificity using the synthesized compounds. For both enzymes, a strong preference for 4-O-methyl glucuronoyl esters rather than unsubstituted glucuronoyl esters was observed. Moreover, we found that α-arylalkyl esters of methyl α-D-glucuronic acid are more easily cleaved by GEs than their corresponding γ-arylalkyl esters. Furthermore, our results suggest a preference of CuGE for glucuronoyl esters of bulky alcohols supporting the suggested biological action of GEs on LCCs. The synthesis of relevant GE model substrates presented here may provide a valuable tool for the screening, selection and development of industrially relevant GEs for delignification of biomass. Biotechnol. Bioeng. 2015;112: 914–922. © 2014 Wiley Periodicals, Inc.
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BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
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Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
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Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.589 SNIP 1.401 CiteScore 4.16
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.621 SNIP 1.425 CiteScore 4.44
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.639 SNIP 1.366 CiteScore 4.04
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.668 SNIP 1.483 CiteScore 4.08
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.538 SNIP 1.357
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.491 SNIP 1.356
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.238 SNIP 1.288
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.368 SNIP 1.362
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.458 SNIP 1.43
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 1.123 SNIP 1.239
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.094 SNIP 1.249
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 1.041 SNIP 1.228
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 1.197 SNIP 1.278
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 1.07 SNIP 1.177
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 1.102 SNIP 1.541
Web of Science (2000): Indexed yes
Scopus rating (1999): SJR 1.511 SNIP 1.567

Original language: English
Enzymatic delignification, Lignin-carbohydrate complexes, Glucuronoyl esterase, Cerrena unicolor, Schizophyllum commune, Substrate specificity
Experimental and Theoretical Mechanistic Investigation of the Iridium-Catalyzed Dehydrogenative Decarbonylation of Primary Alcohols

The mechanism for the iridium-BINAP catalyzed dehydrogenative decarbonylation of primary alcohols with the liberation of molecular hydrogen and carbon monoxide was studied experimentally and computationally. The reaction takes place by tandem catalysis through two catalytic cycles involving dehydrogenation of the alcohol and decarbonylation of the resulting aldehyde. The square planar complex IrCl(CO)(rac-BINAP) was isolated from the reaction between [Ir(cod)Cl](2), rac-BINAP, and benzyl alcohol. The complex was catalytically active and applied in the study of the individual steps in the catalytic cycles. One carbon monoxide ligand was shown to remain coordinated to iridium throughout the reaction, and release of carbon monoxide was suggested to occur from a dicarbonyl complex. IrH2Cl(CO)(rac-BINAP) was also synthesized and detected in the dehydrogenation of benzyl alcohol. In the same experiment, IrHCl2(CO)(rac-BINAP) was detected from the release of HCl in the dehydrogenation and subsequent reaction with IrCl(CO)(rac-BINAP). This indicated a substitution of chloride with the alcohol to form a square planar iridium alkoxo complex that could undergo a beta-hydride elimination. A KIE of 1.0 was determined for the decarbonylation and 1.42 for the overall reaction. Electron rich benzyl alcohols were converted faster than electron poor alcohols, but no electronic effect was found when comparing aldehydes of different electronic character. The lack of electronic and kinetic isotope effects implies a rate-determining phosphine dissociation for the decarbonylation of aldehydes.

General information
State: Published
Organisations: Department of Chemistry, X-ray Crystallography, Organic Chemistry, Stockholm University
Authors: Olsen, E. P. K. (Intern), Singh, T. (Ekstern), Harris, P. (Intern), Andersson, P. G. (Ekstern), Madsen, R. (Intern)
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 13.18 SJR 7.368 SNIP 2.584
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 6.826 SNIP 2.632 CiteScore 12.81
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 6.273 SNIP 2.578 CiteScore 11.92
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 5.953 SNIP 2.455 CiteScore 11.38
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 6.141 SNIP 2.379 CiteScore 10.37
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Facile Large-Scale Synthesis of 5- and 6-Carboxyfluoresceins: Application for the Preparation of New Fluorescent Dyes

A series of fluorescein dyes have been prepared from a common precursor through a very simple synthetic procedure, giving access to important precursors for fluorescent probes. The method has proven an efficient access to regioisomerically pure 5- and 6-carboxyfluoresceins on a large scale, in good yields, and with high regioisomeric purity. Furthermore, we have applied the method to the development of a new type of mixed fluorescein derivatives of 5-carboxyfluorescein. We have demonstrated the scope of the procedure by synthesizing a new type of double chromophore within the fluoro-Jade family.

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry, Department of Micro- and Nanotechnology, Colloids and Biological Interfaces, X-ray Crystallography
Authors: Hammershøj, P. (Intern), Ek, P. K. (Intern), Harris, P. (Intern), Andresen, T. L. (Intern), Clausen, M. H. (Intern)
Number of pages: 10
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Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Facile synthesis of starch-scaffolded bimetallic Au-Pt nanostructure and electrocatalysis

General information
State: Published
Organisations: Department of Chemistry, NanoChemistry, Organic Chemistry
Authors: Engelbrekt, C. (Intern), Seselj, N. (Intern), Ulstrup, J. (Intern), Zhang, J. (Intern)
Number of pages: 1
Publication date: 2015
Main Research Area: Technical/natural sciences
Electronic versions:
Facile_synthesis_of_starch_scaffolded_bimetallic_Au_Pt_nanostructure.pdf

Relations
Activities:
Facile synthesis of starch-scaffolded bimetallic Au-Pt nanostructure and electrocatalysis
Source: PublicationPreSubmission
Source-ID: 118113217
Publication: Research - peer-review › Conference abstract for conference – Annual report year: 2015

Far-Infrared Spectroscopy of Weakly Bound Hydrated Cluster Molecules
The thermodynamic properties of condensed phases, the functionality of many materials and the molecular organization in biological organisms are all governed by the classes of non-covalent interactions that occur already on the microscopic scale between pairs of molecules. A detailed investigation of the intermolecular interactions between prototypical molecular assemblies are valuable for accurate descriptions of larger supramolecular systems such as materials, gas hydrates and biological macromolecules. The aim of this PhD dissertation is to investigate intermolecular interactions for a series of medium-sized molecular clusters with water by means of far-infrared and terahertz neon matrix isolation spectroscopy. The embedding of non-covalent cluster molecules in solid cryogenic neon matrices at 2.8 K ensures a high sensitivity for direct spectroscopic observations of the large-amplitude intermolecular vibrational bands of the cluster molecules in the challenging far-infrared and terahertz spectral regions. A key parameter in the validation of the performance of theoretical predictions for weak non-covalent intermolecular interactions is the dissociation energy $D_0$ that depends heavily on the class of large-amplitude intermolecular vibrational modes for an accurate estimation of the zero-point vibrational energy.

General information
State: Published
Organisations: Department of Chemistry, X-ray Crystallography
Authors: Andersen, J. (Intern), Larsen, R. W. (Intern), Ståhl, K. (Intern)
Number of pages: 184
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Projects:
Far-Infrared Spectroscopy of Weakly Bound Hydrated Cluster Molecules
Source: PublicationPreSubmission
Source-ID: 127352822
Publication: Research › Ph.D. thesis – Annual report year: 2016
FDA-approved small-molecule kinase inhibitors

Kinases have emerged as one of the most intensively pursued targets in current pharmacological research, especially for cancer, due to their critical roles in cellular signaling. To date, the US FDA has approved 28 small molecule kinase inhibitors, half of which were approved in the past 3 years. While the clinical data of these approved molecules are widely presented and structure–activity relationship (SAR) has been reported for individual molecules, an updated review that analyzes all approved molecules and summarizes current achievements and trends in the field has yet to be found. Here we present all approved small-molecule kinase inhibitors with an emphasis on binding mechanism and structural features, summarize current challenges, and discuss future directions in this field.

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry, Center for Nanomedicine and Theranostics, Novo Nordisk A/S
Authors: Wu, P. (Intern), Nielsen, T. E. (Ekstern), Clausen, M. H. (Intern)
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BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): SJR 5.218 SNIP 2.933 CiteScore 9.77
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 5.385 SNIP 3.053 CiteScore 9.77
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 5.032 SNIP 2.789 CiteScore 9.1
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 5.362 SNIP 2.685 CiteScore 10.19
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 5.015 SNIP 2.744 CiteScore 10.74
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 5.36 SNIP 2.599 CiteScore 10.75
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 5.434 SNIP 2.52
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 4.921 SNIP 2.456
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 4.623 SNIP 2.357
Scopus rating (2007): SJR 4.453 SNIP 2.48
Scopus rating (2006): SJR 4.325 SNIP 2.524
Scopus rating (2005): SJR 4.173 SNIP 2.564
Scopus rating (2004): SJR 3.739 SNIP 2.753
Scopus rating (2003): SJR 3.782 SNIP 2.637
Scopus rating (2002): SJR 3.888 SNIP 2.694
Scopus rating (2001): SJR 4.238 SNIP 2.847
Scopus rating (2000): SJR 4.593 SNIP 3.17
Further iridoid glucosides in the genus Manulea (Scrophulariaceae).

From Manulea altissima (Scrophulariaceae) were isolated five known secoiridoid glucosides sweroside, eustomoside, eustoside, secoxyloganin and secologanoside as well as the 4″-O-rhamnopyranosyl-feruloyl ester of adoxosidic acid, named altissimoside. Also, the caffeoyl phenylethanoid glycoside verbascoside was isolated. In addition two previously unknown terpenoid esters of 6β-hydroxy 8-epi-boschnaloside, named manucoside A and B were isolated from a formerly obtained fraction from the work-up of Manulea corymbosa. The distribution of iridoid glucosides in the Scrophulariaceae is discussed.

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Organisations: Department of Chemistry, Organic Chemistry, The Royal Botanic Gardens
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Publication information
Journal: Phytochemistry
Volume: 109
ISSN (Print): 0031-9422
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
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BFI (2016): BFI-level 1
Scopus rating (2016): SJR 1.101 SNIP 1.372 CiteScore 3.18
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.897 SNIP 1.392 CiteScore 3
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.127 SNIP 1.56 CiteScore 3.07
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.088 SNIP 1.679 CiteScore 3.63
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.164 SNIP 1.785 CiteScore 3.52
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.024 SNIP 1.642 CiteScore 3.37
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
Genotype-Property Patient-Phenotype Relations Suggest that Proteome Exhaustion Can Cause Amyotrophic Lateral Sclerosis

Late-onset neurodegenerative diseases remain poorly understood as search continues for the perceived pathogenic protein species. Previously, variants in Superoxide Dismutase 1 (SOD1) causing Amyotrophic Lateral Sclerosis (ALS) were found to destabilize and reduce net charge, suggesting a pathogenic aggregation mechanism. This paper reports analysis of compiled patient data and experimental and computed protein properties for variants of human SOD1, a major risk factor of ALS. Both stability and reduced net charge correlate significantly with disease, with larger significance than previously observed. Using two independent methods and two data sets, a probability <3% (t-statistical test) is found that ALS-causing mutations share average stability with all possible 2907 SOD1 mutations. Most importantly, un-weighted patient survival times correlate strongly with the misfolded/unfolded protein copy number, expressed as an exponential function of the experimental stabilities ($R^2 = 0.31, p = 0.002$), and this phenotype is further aggravated by charge ($R^2 = 0.51, p = 1.8 \times 10^{-5}$). This finding suggests that disease relates to the copy number of misfolded proteins. Exhaustion of motor neurons due to expensive protein turnover of misfolded protein copies is consistent with the data but can further explain e.g. the expression-dependence of SOD1 pathogenicity, the lack of identification of a molecular toxic mode, elevated SOD1 mRNA levels in sporadic ALS, bioenergetic effects and increased resting energy expenditure in ALS patients, genetic risk factors affecting RNA metabolism, and recent findings that a SOD1 mutant becomes toxic when proteasome activity is recovered after washout of a proteasome inhibitor. Proteome exhaustion is also consistent with energy-producing mitochondria accumulating at the neuromuscular junctions where ALS often initiates. If true, this exhaustion mechanism implies a complete change of focus in treatment of ALS towards actively nursing the energy state and protein turnover of the motor neurons.

General information
State: Published
Organisations: Department of Chemistry, Physical and Biophysical Chemistry
Authors: Kepp, K. P. (Intern)
Number of pages: 19
Primates Mammalia Vertebrata Chordata Animalia (Animals, Chordates, Humans, Mammals, Primates, Vertebrates) -
Hominidae [86215] human common middle age female, male, Human SOD1 gene [Hominidae], mRNA, Proteasome
140879-24-9 EC 3.4.25.1, RNA metabolism, SOD1 expression mutation, 02506, Cytology - Animal, 02508, Cytology -
Human, 03502, Genetics - General, 03506, Genetics - Animal, 03508, Genetics - Human, 10062, Biochemistry studies -
Nucleic acids, purines and pyrimidines, 10064, Biochemistry studies - Proteins, peptides and amino acids, 10802,
Enzymes - General and comparative studies: coenzymes, 12502, Pathology - General, 17506, Muscle - Pathology,
20504, Nervous system - Physiology and biochemistry, 20506, Nervous system - Pathology, 34508, Immunology -
Immunopathology, tissue immunology, Clinical Immunology, Molecular Genetics, Neurology, Amyotrophic lateral sclerosis
Amyotrophic Lateral Sclerosis (MeSH) nervous system disease, muscle disease pathology, Genotype-property, Protein
copy number, Proteome, Resting energy expendi- ture, Biochemistry and Molecular Biophysics, Human Medicine, Medical
Sciences, Motor neuron nervous system, Neuromuscular junction nervous system, 2C9V Protein Data Bank amino acid
sequence, Multidisciplinary, Human Superoxide-dismutase, Wild-type Sod1, Mutant Sod1, Stability changes, Motor-
neurons, Mouse model, HEXANUCLEOTIDE REPEAT, DISEASE PROGRESSION, FAMILIAL ALS, Mutations
Graphene-supported platinum catalysts for fuel cells

Increasing concerns with non-renewable energy sources drive research and development of sustainable energy technology. Fuel cells have become a central part in solving challenges associated with energy conversion. This review summarizes recent development of catalysts used for fuel cells over the past 15 years. It is focused on polymer electrolyte membrane fuel cells as an environmentally benign and feasible energy source. Graphene is used as a promising support material for Pt catalysts. It ensures high catalyst loading, good electrocatalysis and stability. Attention has been drawn to structural sensitivity of the catalysts, as well as polymetallic and nanostructured catalysts in order to improve the oxygen reduction reaction. Characterization methods including electrochemical, microscopic and spectroscopic techniques are summarized with an overview of the latest technological advances in the field. Future perspective is given in a form of Pt-free catalysts, such as microbial fuel cells for long-term development.

Halide Binding and Inhibition of Laccase Copper Clusters: The Role of Reorganization Energy

Laccase-like proteins are multicopper oxidases involved in several biological and industrial processes. Their application is commonly limited due to inhibition by fluoride and chloride, and as-isolated proteins are often substantially activated by heat, suggesting that multiple redox states can complicate characterization. Understanding these processes at the molecular level is thus desirable but theoretically unexplored. This paper reports systematic calculations of geometries, reorganization energies, and ionization energies for all partly oxidized states of the trinuclear copper clusters in realistic models with similar to 200 atoms. Corrections for scalar-relativistic effects, dispersion, and thermal effects were estimated. Fluoride, chloride, hydroxide, or water was bound to the T2 copper site of the oxidized resting state, and the peroxo intermediate was also computed for reference. Antiferromagnetic coupling, assigned oxidation states, and general structures were consistent with known spectroscopic data. The computations show that (i) ligands bound to the T2 site substantially increase the reorganization energy of the second reduction of the resting state and reduce the redox potentials, providing a possible mechanism for inhibition; (ii) the reorganization energy is particularly large for F- but also high for Cl-, consistent with the experimental tendency of inhibition; (iii) reduction leads to release of Cl- from the T2 site, suggesting a mechanism for heat/reduction activation of laccases by dissociation of inhibiting halides or hydroxide from...
General information
State: Published
Organisations: Department of Chemistry, Physical and Biophysical Chemistry
Authors: Kepp, K. P. (Intern)
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Publication information
Journal: INORGANIC CHEMISTRY
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Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 4.64 SJR 1.774 SNIP 1.198
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.805 SNIP 1.239 CiteScore 4.7
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.869 SNIP 1.314 CiteScore 4.69
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.819 SNIP 1.379 CiteScore 4.9
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 2.08 SNIP 1.35 CiteScore 4.72
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.952 SNIP 1.373 CiteScore 4.64
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.98 SNIP 1.323
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.982 SNIP 1.47
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 2.025 SNIP 1.412
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 2.136 SNIP 1.544
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.828 SNIP 1.508
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 2.012 SNIP 1.46
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 › Journal article – Annual report year: 2015

Highly Selective Liquid-Phase Benzylation of Anisole with Solid-Acid Zeolite Catalysts
Zeolites were evaluated as solid acid catalysts for the liquid-phase benzylation of anisole with benzyl alcohol, benzyl bromide, and benzyl chloride at 80 °C. Among the examined zeolites, H-mordenite-10 (H-MOR-10) demonstrated particular high activity (>99 %) and excellent selectivity (>96 %) to the monobenzylated products, ortho/para benzyl anisole, using benzyl alcohol as reagent (anisole/alcohol molar ratio = 28). Analogous reactions with benzyl halides resulted in lower yields of the desired monobenzylated products. The conversion of benzyl alcohol was confirmed to be proportional to the amount of added H-MOR-10, and the linear free-energy relationship relating the conversion of substituted benzyl alcohol and substituent constants as well as the orientation effect of substituents of anisole on the
distribution of ortho/para/meta isomers was evaluated.

**General information**

*State:* Published  
*Organisations:* Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry  
*Authors:* Poreddy, R. (Intern), Shunmugavel, S. (Intern), Riisager, A. (Intern)  
*Number of pages:* 9  
*Pages:* 1053-1061  
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**Publication information**

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BFI (2016): BFI-level 1  
Scopus rating (2016): CiteScore 2.55 SJR 0.974 SNIP 0.878  
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  
Scopus rating (2009): SJR 1.269 SNIP 0.907  
Web of Science (2009): Indexed yes  
BFI (2008): BFI-level 2  
Scopus rating (2008): SJR 1.225 SNIP 1.015  
Web of Science (2008): Indexed yes  
Scopus rating (2007): SJR 1.522 SNIP 1.382  
Web of Science (2007): Indexed yes  
Scopus rating (2006): SJR 1.59 SNIP 1.202  
Web of Science (2006): Indexed yes  
Scopus rating (2005): SJR 1.444 SNIP 1.17
Hofmeister effect of salt mixtures on thermo-responsive poly(propylene oxide)

The Hofmeister series is a classification of ions regarding their ability to stabilize or destabilize aqueous solutions of proteins, polymers and other molecules which are partly miscible with water. In this study, we employ differential scanning calorimetry to investigate how the stability of aqueous solutions of poly(propylene oxide) is affected by mixtures of ions with different location in the Hofmeister series. Our results show that the Hofmeister effects of pure salt species are not always linearly additive and that the relative effect of some ions can be reversed depending on the composition of the salt mixture as well as by the absolute and relative concentration of the different species. We suggest that these results can lead to a better understanding of the potential role of the Hofmeister effect in regulation of biological processes, which does always take place in salt mixtures rather than solutions containing just single salt species.
Hydrogen evolution at nanoporous gold/tungsten sulfide composite film and its optimization

Development of efficient and economical electrochemical systems for water splitting is a key part of renewable energy technology. Amorphous films of tungsten sulfide have been deposited by electrochemical reduction of tetrathiotungstate ions (WS$_4^{2-}$) on dealloyed nanoporous gold (NPG) for electrochemical hydrogen evolution reaction (HER). The electrocatalytic performance has been proved to be sensitive to the thickness of the deposited layer, with an optimal deposition time of 600 s identified. The bi-continuous nanoporous morphology of the composites has been confirmed by transmission electron microscopy (TEM), and is beneficial for high exposure of catalytic sites and electrolyte access to the electrode surface. High-resolution TEM (HRTEM) has been employed to characterize the strong adhesion between the ultrathin film (less than 1 nm) and gold skeleton, allowing rapid charge transfer and long-term stability. The measured Tafel slope of 74 mV dec$^{-1}$ implies an underlying Volmer-Heyrovsky HER mechanism.

General information

State: Published
Hydrogen Production by Homogeneous Catalysis: Alcohol Aceptorless Dehydrogenation

The lifestyle in the modern western world is highly depending on the accessibility of energy and bulk chemicals. Energy is needed in the transportation sector, but also domestic and industrial consumptions of energy is comprehensive. Bulk chemicals are probably more important than people realize, and are fundamental for the thrive of almost all business fields. The latter include the industries of agriculture, food additives, pharmaceuticals, electronics, plastic, fragrances, and more. Today, the major source of both energy and bulk chemicals is fossil fuels, being responsible for more than 80 % of the energy supplies. The large amounts of CO₂ release owing to fossil fuel usage is believed to cause global warming on the long term, a highly undesired environmental consequence. Hence, it is of critical importance that alternative sources are developed and implemented in the society. One suggested solution for the energy sector is the application of a hydrogen economy, which transform the chemical energy in water and/or biomass into hydrogen. Considered as an energy carrier, hydrogen is then transported to the site of use where fuel cells convert its chemical energy into electricity.Here, we review the progress in hydrogen production from biomass using homogeneous catalysis. Homogeneous catalysis has the advance of generally performing transformations at much milder conditions than traditional heterogeneous catalysis, and hence it constitutes a promising tool for future applications for a sustainable energy sector. In particular, only alcohol containing substances are covered. As such, alcohol acceptorless dehydrogenation (AAD) is the main topic of this review. Moreover, it is more easily investigated for eluding mechanistic property. This review is divided up in four main chapters according to substrates. The first chapter, Model Substrates, describes the development of alcohol acceptorless dehydrogenation using substrates that can be categorized as model substrates. This includes e.g. isopropanol. The second chapter, Substrates with Synthetic Applications, deals with synthetic applications of alcohol acceptorless dehydrogenation. The third chapter, Biorelevant Substrates, concentrates on the use of alcohols such as ethanol, which are biomass related. The topic is alcohol acceptorless dehydrogenation reactions for both H₂ production and the concurrent synthetic application. Finally, Chap. 4, Substrates for H₂ Storage, is focusing on the use of alcohol acceptorless dehydrogenation of alcohols relevant as future H₂ storage molecules. This is in particular methanol.
Induced sclerotium formation exposes new bioactive metabolites from Aspergillus sclerotiocarbonarius

Sclerotia are known to be fungal survival structures, and induction of sclerotia may prompt production of otherwise undiscovered metabolites. Aspergillus sclerotiocarbonarius (IBT 28362) was investigated under sclerotium producing conditions, which revealed a highly altered metabolic profile. Four new compounds were isolated from cultivation under sclerotium formation conditions and their structures elucidated using different analytical techniques (HRMS, UV, 1D and 2D NMR). This included sclerolizine, an alkylated and oxidized pyrrolizine, the new emindole analog emindole SC and two new carbonarins; carbonarins I and J. We have identified the three latter as true sclerotial metabolites. All metabolites were tested for antifungal and antiinsectan activity, and sclerolizine and carbonarin I displayed antifungal activity against Candida albicans, while all four showed antiinsectan activity. These results demonstrate induction of sclerotia as an alternative way of triggering otherwise silent biosynthetic pathways in filamentous fungi for the discovery of novel bioactive secondary metabolites.
Injectable Colloidal Gold for Use in Intrafractional 2D Image-Guided Radiation Therapy

In the western world, approximately 50% of all cancer patients receive radiotherapy alone or in combination with surgery or chemotherapy. Image-guided radiotherapy (IGRT) has in recent years been introduced to enhance precision of the delivery of radiation dose to tumor tissue. Fiducial markers are often inserted inside the tumor to improve IGRT precision and to enable monitoring of the tumor position during radiation therapy. In the present article, a liquid fiducial tissue marker is presented, which can be injected into tumor tissue using thin and flexible needles. The liquid fiducial has high radio-opacity, which allows for marker-based image guidance in 2D and 3D X-ray imaging during radiation therapy. This is achieved by surface-engineering gold nanoparticles to be highly compatible with a carbohydrate-based gelation matrix. The new fiducial marker is investigated in mice where they are highly biocompatible and stable after implantation. To investigate the clinical potential, a study is conducted in a canine cancer patient with spontaneous developed solid tumor in which the marker is successfully injected and used to align and image-guide radiation treatment of the canine patient. It is concluded that the new fiducial marker has highly interesting properties that warrant investigations in cancer patients.
In Situ Spectroscopic Investigation of the Rhenium-Catalyzed Deoxydehydration of Vicinal Diols

The mechanism of the CH₃ReO₃-catalyzed deoxydehydration of a vicinal diol to an alkene driven by oxidation of a secondary alcohol was investigated by time-resolved, in situ IR spectroscopy and was found to occur in three steps: 1) reduction of the catalytically active methyltrioxorhenium(VII) to a rhenium(V) complex (the rate-limiting step), 2) condensation of the diol and the rhenium(V) complex to a rhenium(V) diolate, and 3) extrusion of the alkene accompanied by oxidation of the Re center and thus regeneration of CH₃ReO₃. The reaction follows zero-order kinetics initially but, unexpectedly, accelerates towards the end, which is explained in terms of a deactivating pre-equilibrium, in which the catalytically active CH₃ReO₃ condenses reversibly with the diol to form an inactive rhenium(VII) diolate. This conclusion is supported by the direct observation of a catalytically inactive species as well as DFT calculations of the IR spectra of the relevant compounds.

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Authors: Dethlefsen, J. R. (Intern), Fristrup, P. (Intern)
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Integration of CO$_2$ air capture and solid oxide electrolysis for methane production

This work studied the production of substitute natural gas (SNG) from CO$_2$ captured from the atmosphere followed by co-electrolysis with H$_2$O in solid oxide electrolyzer cells (SOEC) and downstream catalytic methane production. Over the coming 20 years, Denmark is on a track to remove fossil fuels from all sectors of the energy system except for transportation. In the recently published Energikoncept 2035 [1], the Danish grid operator, Energinet.dk lays out a scenario based on 72% wind power and 21% biomass and waste in the electricity grid mix. In this scenario, biogas and electrolysis gasses are projected to be used for production of process heat, peak-load power generation and on the longer term to replace hydrocarbons in the most energy intensive parts of the transportation sector, especially aviation. As a prerequisite for the scenario, no biomass can be imported to enhance the supply of combustible resources. In such an energy system, technologies for production of CO$_2$ neutral hydrocarbons for easy storage and use in the existing infrastructure; especially in the natural gas grid; may be of great value. The studied technology fulfills those demands. The main goal of the work was to design a plant and develop a thermodynamic model of the plant operation, enabling analyses related to selection of operating parameters; analysis and optimization of internal heat recovery and integration between the main technological subsystems. Finally to identify the main areas of technological development through economic analyses. The work included experimental work on an example of a system for capture of CO$_2$: the humidity swing (HS) system, qualitatively evaluating the H$_2$O uptake and CO$_2$ desorption characteristics of the sorbent material, especially in relation to the supply of H$_2$O to the sorbent. It was found that H$_2$O supplied in the gas phase resulted in slow uptakes and desorption rates of CO$_2$ whereas supplying liquid water to the sorbent resulted in fast desorption in the first hours, after which the rate dropped sharply. A method was developed and used to characterize the impurities present in CO$_2$ stream from the HS system in addition to the temperature vacuum swing (TVS) system under development by Climeworks Ltd. The method relied on adsorption of impurities on a filter consisting of nickel-yttria-stabilised-zirconia (Ni/YSZ), similar to the material used in the fuel electrodes of SOECs followed by elemental analysis by glow discharge mass spectrometry. The method had a sub-ppm detection limit. Across the tested systems, a range of elements known to be detrimental to solid oxide cell (SOC) operation were detected in the range from tens of ppb to 20 ppm. The SNG plant was modelled using the process integration software package PRO/II alongside the design process, and a series of minor studies using PRO/II and thermodynamic analysis software FactSage® aided the design process. This included studying a long range of questions such as alternative strategies for CO$_2$ compression; the structure of the methanation plant; and the risk of carbon formation in both SOEC and methanation reactors, etc. The model was based on a thermodynamic 0-dimensional model of the electrolyzer sub-system, developed to technological specifications from the thermodynamic SOEC model published by Sun et al. [2] This model was used for a study of operating parameters, and two design cases were identified for the full plant based on these results. The two cases both operated at 80 atm, and had SOEC operating temperatures of 850 °C and 600 °C. The area specific resistance (ASR) of the SOECs were extrapolated to high pressure and low temperatures based on data for standard DTU Energy Ni-YSZ based cells, and the pressure dependency of the individual cell processes. With the full plant model finished, the potential for internal recovery of surplus heat was analyzed, and a network of heat exchangers synthesized in order to minimize the requirements for external heating and cooling services. Based on the process flow sheets and the heat exchanger network, the dimensions and costs of the equipment of the plant were calculated and additional cost components such as installation of equipment, land use, labor costs, operation and maintenance, etc. were estimated according to standard methods. The plant had a yearly production capacity of
575,000 Nm3 of SNG with a methane content above 98.5 % which resulted in a Wobbe index of 49 MJ/Nm3 which is sufficient for injection into the natural gas grid. The SOEC stack power was around 700 kW, and the plant operated a tan energy efficiency of 65 % (HHV) and 58 % (LHV). An economic analysis based on guidelines from the Danish energy agency and standard methods was conducted accounting for interest rates, taxes, depreciation etc. at a minimum acceptable rate of return set to the minimum of 4 %. The economic analysis resulted in SNG production prices of 1.88 €/Nm3 and 2.94 €/Nm3 based on an electricity price of 18.6 €/MJ, a price of process heat at 120 °C of 11.9 €/MJ and a price of cell area of 0.23 €/cm2. The main cost drivers were identified as the capital costs of the SOEC and air capture systems and the heat exchanger network. For operating costs, the electricity price had a significant impact, whereas the dependency of the SNG price on the heat price was minor. The technical issues where discussed in separate chapters interspersed by chapters documenting the modelling and design process. Finally, a comprehensive discussion at the end treats the technical issues of the plant in the light of the economic analysis.
secondary-branched butanethiol (25 %) and near that for linear-chain 1-butanol (33 %).

**General information**

- **State:** Published
- **Organisations:** NanoChemistry, Department of Chemistry, Organic Chemistry, University of Sydney, Xiamen University, Chinese Academy of Sciences, Shanghai University
- **Authors:** Ouyang, R. (Ekstern), Yan, J. (Intern), Jensen, P. S. (Intern), Asic, E. (Intern), Gan, S. (Intern), Tanner, D. A. (Intern), Mao, B. (Ekstern), Niu, L. (Ekstern), Zhang, J. (Intern), Tang, C. (Ekstern), Hush, N. S. (Ekstern), Reimers, J. R. (Ekstern), Ulstrup, J. (Intern)
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  - Scopus rating (2014): SJR 1.362 SNIP 0.905 CiteScore 3.12
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  - Scopus rating (2013): SJR 1.442 SNIP 0.948 CiteScore 3.22
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  - Scopus rating (2012): SJR 1.763 SNIP 0.955 CiteScore 3.24
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  - BFI (2011): BFI-level 2
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  - BFI (2010): BFI-level 2
  - Scopus rating (2010): SJR 1.872 SNIP 1.031
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  - Scopus rating (2009): SJR 1.91 SNIP 1.12
  - Web of Science (2009): Indexed yes
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  - Scopus rating (2008): SJR 2.153 SNIP 1.098
  - Scopus rating (2007): SJR 2.215 SNIP 1.129
  - Web of Science (2007): Indexed yes
  - Scopus rating (2006): SJR 2.008 SNIP 1.159
  - Web of Science (2006): Indexed yes
  - Scopus rating (2005): SJR 2.067 SNIP 1.147
Investigation of a 6-MSA Synthase Gene Cluster in Aspergillus aculeatus Reveals 6-MSA-derived Aculinic Acid, Aculins A-B and Epi-Aculin A

Aspergillus aculeatus, a filamentous fungus belonging to the Aspergillus clade Nigri, is an industrial workhorse in enzyme production. Recently we reported a number of secondary metabolites from this fungus; however, its genetic potential for the production of secondary metabolites is vast. In this study we identified a 6-methylsalicylic acid (6-MSA) synthase from A. aculeatus, and verified its functionality by episomal expression in A. aculeatus and heterologous expression in A. nidulans. Feeding studies with fully $^{13}$C-labeled 6-MSA revealed that 6-MSA is incorporated into aculinic acid, which further incorporates into three compounds that we name aculins A and B, and epi-aculin A, described here for the first time. Based on NMR data and bioinformatic studies we propose the structures of the compounds as well as a biosynthetic pathway leading to formation of aculins from 6-MSA.

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Scopus rating (2016): CiteScore 2.64 SJR 1.242 SNIP 0.733
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.255 SNIP 0.748 CiteScore 2.77
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.386 SNIP 0.852 CiteScore 2.88
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Scopus rating (2013): SJR 1.622 SNIP 0.849 CiteScore 3.15
Investigation of L(+)-Ascorbic Acid with Raman Spectroscopy in Visible and UV Light

Abstract: Raman spectroscopy investigations of L(+)-ascorbic acid and its mono- and di-deprotonated anions (AH(-) and A(2-)) are reviewed and new measurements reported with several wavelengths, 229, 244, 266, 488, and 532nm. Results are interpreted, assisted by new DFT/B3LYP quantum chemical calculations with 6-311++G(d,p) basis sets for several conformations of ascorbic acid and the anions. Raman spectra were measured during titration with NaOH base in an oxygen-poor environment to avoid fluorescence when solutions were alkaline. The ultraviolet (UV) absorption band for ascorbic acid in aqueous solution at similar to 247nm was found to cause strong resonance enhancement for the ring C-C stretching mode (called B) at similar to 1692cm(-1). The ascorbate mono-anion absorbs at similar to 264.8nm giving Raman resonance enhancement for the same ring C-C bond stretching, downshifted to similar to 1591cm(-1). Finally, for the ascorbate di-anion, absorption was found at similar to 298.4nm with molar absorptivity of similar to 7,000 L mol(-1) cm(-1) and below similar to 220nm. With UV light (244 and 266nm), strongly basic solutions gave pronounced Raman resonance enhancement at similar to 1556cm(-1). Relatively weak preresonance enhancement was seen for A(2-) when excitation was done with 229nm UV light, allowing water bands to become observable as for normal visible light Raman spectra.
Ascorbate, Ascorbic acid, Conformation, DFT calculation, Raman spectroscopy, X-ray structure

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Iridoid glucosides in the endemic Picconia azorica (Oleaceae)

In our continued investigation of plants from the family Oleaceae we have now investigated Picconia azorica endemic to the Azores. Like most species within the family it contains the oleoside-based secoiridoid glucosides ligstroside and oleuropein as the main compounds and in addition verbascoside and echinacoside. As with the previously investigated Picconia excelsa, it also contained the carbocyclic iridoid glucosides involved in the biosynthetic pathway to the oleoside derivatives. However, while P. excelsa contained loganin esterified with some monoterpenoid acids, P. azorica contains similar esters of 7-epi-loganic acid named Picconioside A and B. In addition were found the two 7-O-E/Z-cinnamoyl esters of 7-epi-loganic acid named Picconioside C and D.

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Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.127 SNIP 1.56 CiteScore 3.07
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.088 SNIP 1.679 CiteScore 3.63
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.164 SNIP 1.785 CiteScore 3.52
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.024 SNIP 1.642 CiteScore 3.37
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.132 SNIP 1.66
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.055 SNIP 1.539
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.052 SNIP 1.473
Web of Science (2008): Indexed yes
Isomerization of Orthogonal Molecular Switches Encapsulated within Micelles Solubilizing Carbon Nanotubes

We study the effects of the proximity of the orthogonal dipole-switching moiety dihydroazulene/vinylheptafulvene (DHA/VHF) to carbon nanotubes (CNTs). The switches are introduced into a micelle surrounding the CNTs, thereby achieving very close proximity between the molecules and the CNTs for the first time. The change of the molecules' configuration is not hindered by its encapsulation: We report the reversible switching of molecules inside CNT surrounding micelles. The orthogonality of the switch also allows us for the first time to observe the effect of the molecule on the emission spectra of the CNTs and the resulting reversible redshift of the nanotubes' emission by the change of the molecules' conformation.

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Scopus rating (2016): CiteScore 4.48 SJR 1.948 SNIP 1.181
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Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Ketene as a Reaction Intermediate in the Carbonylation of Dimethyl Ether to Methyl Acetate over Mordenite

Unprecedented insight into the carbonylation of dimethyl ether over Mordenite is provided through the identification of ketene (CH₂CO) as a reaction intermediate. The formation of ketene is predicted by detailed DFT calculations and verified experimentally by the observation of doubly deuterated acetic acid (CH₂DCOOD), when D₂O is introduced in the feed during the carbonylation reaction.

General information

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Organisations: Department of Chemical and Biochemical Engineering, CHEC Research Centre, Center for Atomic-scale Materials Design, Department of Physics, Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Haldor Topsoe AS, SUNCAT Center for Interface Science and Catalysis
Authors: Rasmussen, D. B. (Intern), Christensen, J. M. (Intern), Temel, B. (Intern), Studt, F. (Intern), Moses, P. G. (Intern), Rossmeisl, J. (Intern), Riisager, A. (Intern), Jensen, A. D. (Intern)
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Ketene as a Reaction Intermediate in the Carbonylation of Dimethyl Ether to Methyl Acetate over Mordenite
Unprecedented insight into the carbonylation of dimethyl ether over Mordenite is provided through the identification of ketene (CH₂CO) as a reaction intermediate. The formation of ketene is predicted by detailed DFT calculations and verified experimentally by the observation of doubly deuterated acetic acid (CH₂DCOOD), when D₂O is introduced in the feed during the carbonylation reaction.
Kinetic Isotope Effects (KIE) and Density Functional Theory (DFT): A Match Made in Heaven?

Determination of experimental kinetic isotope effects (KIE) is one of the most useful tools for the exploration of reaction mechanisms in organometallic chemistry. The approach has been further strengthened during the last decade with advances in modern computational chemistry. This allows for the calculation of a theoretical KIE that can often be compared directly to the experimental value. This combined experimental/theoretical approach can be particularly useful in cases where the value of the experimental KIE is not directly associated with one particular reaction step (e.g., in a catalytic reaction). The approach is highlighted by using recent examples from both stoichiometric and catalytic reactions, homogeneous and heterogeneous catalysis, and enzyme catalysis to illustrate the expected accuracy and utility of this approach.

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Scopus rating (2014): SJR 0.956 SNIP 0.574 CiteScore 2.09
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Scopus rating (2013): SJR 1.017 SNIP 0.567 CiteScore 2.08
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BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.137 SNIP 0.623 CiteScore 2.1
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.288 SNIP 0.664 CiteScore 2.43
ISI indexed (2011): ISI indexed yes
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BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.214 SNIP 0.63
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.261 SNIP 0.685
Web of Science (2009): Indexed yes
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Scopus rating (2008): SJR 1.465 SNIP 0.728
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Lignin Valorization by Heterogeneous Catalytic Oxidation

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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)
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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 2. These monomers are connected with various linkages with the most common one being the β-O-4 linkage 3. 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 4. 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 form oxidation of side chain. The products we obtained in these reactions are based on the severity of the reaction conditions 4. Here, we therefore present an overview of the recent research about conversion of some lignin model compounds using heterogeneous catalysis in oxidation reactions.

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LSM Microelectrodes: Kinetics and Surface Composition

Lanthanum strontium manganite microelectrodes with the nominal composition of (La0.75Sr0.25)0.95MnO3 and a thickness of ca 500 nm was electrochemically characterized in situ at temperatures from 660 to 850 °C using a controlled atmosphere high temperature scanning probe microscope. Impedance spectroscopy and cyclic voltammetry were performed on electrodes with diameters of 20–100 μm in oxygen, air and nitrogen both at open circuit voltage and at anodic and cathodic polarization. In situ conductance mapping, ex situ surface analysis by time-of-flight secondary ion mass spectrometry, and scanning electron microscopy were performed to observe electrical, chemical and structural changes on the microelectrodes. © 2015 The Electrochemical Society.
Manipulation of molecular vibrational motions via pure rotational excitations

The coupling between different molecular degrees of freedom plays a decisive role in many quantum phenomena, including electron transfer and energy redistribution. Here, we demonstrate a quantum-mechanical time-dependent simulation to explore how a vibrational motion in a molecule can be affected via the rotation-vibration coupling. Our simulations show that a slow (compared to the vibrational period) rotational excitation leads to a smooth increase in the bond length whereas a fast rotational excitation leads to a non-stationary vibrational motion.

Mechanistic insights into the oxidative dehydrogenation of amines to nitriles in continuous flow

The oxidative dehydrogenation of various aliphatic amines to their corresponding nitrile compounds using RuO$_2$/Al$_2$O$_3$ catalysts in air was successfully applied to a continuous flow reaction. Conversions of amines (up to >99%) and yields of nitriles (up to 77%) varied depending on reaction conditions and the amine utilised. The presence of water was found to be important for the activity and stability of the RuO$_2$/Al$_2$O$_3$ catalyst. The Hammett relationship and in situ infrared spectroscopy were applied to divulge details about the catalytic mechanism of the oxidative dehydrogenation of amines.
Membrane Interaction of the Factor VIIIa Discoidin Domains in Atomistic Detail

A recently developed membrane-mimetic model was applied to study membrane interaction and binding of the two anchoring C2-like discoidin domains of human coagulation factor VIIIa (FVIIIa), the C1 and C2 domains. Both individual domains, FVIII C1 and FVIII C2, were observed to bind the phospholipid membrane by partial or full insertion of their extruding loops (the spikes). However, the two domains adopted different molecular orientations in their membrane-bound states; FVIII C2 roughly was positioned normal to the membrane plane, while FVIII C1 displayed a multitude of tilted orientations. The results indicate that FVIII C1 may be important in modulating the orientation of the FVIIIa molecule to optimize the interaction with FIXa, which is anchored to the membrane via its γ-carboxyglutamic acid-rich (Gla) domain. Additionally, a structural change was observed in FVIII C1 in the coiled main chain leading the first spike. A tight interaction with one lipid per domain, similar to what has been suggested for the homologous FVa C2, is characterized. Finally, we rationalize known FVIII antibody epitopes and the scarcity of documented hemophilic missense mutations related to improper membrane binding of FVIIIa, based on the prevalent nonspecificity of ionic interactions in the simulated membrane-bound states of FVIII C1 and FVIII C2.
Membrane technologies for water treatment and reuse in the textile industry

Textile wastewater is a challenging feed stream for treatment by membrane separation because of its complex composition and the presence of reactive components. Here we briefly present examples of reverse osmosis-, nanofiltration- and ultrafiltration-based systems as well as membrane bioreactor technology for textile wastewater remediation. However, for all of these approaches the general issue of (bio)fouling represents a major obstacle for full-scale industrial implementation. Forward osmosis (FO) membranes have recently attracted considerable interest because the low fouling propensity of FO membranes makes them an intriguing supplement to existing methods. We present the FO principle with some current FO membrane developments including biomimetic aquaporin FO membranes, and exemplify how they can be used to concentrate textile dyes.

General information
State: Published
Organisations: Department of Physics, Department of Environmental Engineering, Urban Water Engineering, Department of Chemistry, University of Maribor
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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 to isolate 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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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.

Microwave-assisted synthesis of graphene-Prussian Blue networked nanocomposites for electrocatalysis

There has been a great deal of interest recently in Prussian blue functional graphene. Due to displayed advantage of both Prussian blue and graphene, we presented a one-pot and green method to synthesize interlocked graphene-Prussian Blue nanocomposites. Considering that graphene oxide (GO) has shown the property as electron acceptor, Fe$^{2+}$ as reduced agent was applied to reduce GO without toxic group in low temperature and under mild environment, high quality Prussian blue cube without coordinated water was prepared and in same step. Reduce graphene oxide was functionalized by high Prussian blue cube in reduced process, and high quality Prussian blue cubes are easily combined with rGO by chemical bond, it shown more stable and highly distribute. Obtained reduced graphene oxide–PB composite (rGO-PB) was characterized by UV-vis, XRD, Raman, SEM, TEM, and electrochemistry method. This kind materials displaying high performance when was used for electrocatalytic reduction H$_2$O$_2$.

MnFe/Al$_2$O$_3$ Catalyst Synthesized by Deposition Precipitation for Low-Temperature Selective Catalytic Reduction of NO with NH$_3$

Mn-Fe/Al$_2$O$_3$ and Mn-Fe/TiO$_2$ catalysts have been prepared by impregnation (IMP) and deposition precipitation (DP) and characterized with several techniques including: XRDP, N$_2$-physisorption, NH$_3$-TPD, H$_2$-TPR, TGA and XPS. 40 wt% Mn$_{0.75}$Fe$_{0.25}$/Al$_2$O$_3$ prepared with ammonia carbamate as precipitating agent showed the same superior low temperature selective catalytic reduction of NO with NH$_3$ as did 25 wt% Mn$_{0.75}$Fe$_{0.25}$/TiO$_2$ prepared in the same way. Both catalysts were much more active when prepared by DP instead of IMP. 25 wt% Mn$_{0.75}$Fe$_{0.25}$/TiO$_2$ and 40 wt% Mn$_{0.75}$Fe$_{0.25}$/Al$_2$O$_3$ prepared by DP were exposed to a gas containing 20 vol% H$_2$O at temperatures between 140 and 200 °C degrees C and compared to an industrial V$_2$O$_5$-WO$_3$ catalyst tested at 220 °C. Both homemade catalysts were severely inhibited by 20 vol% H$_2$O$_2$. However, used at 180 °C they match the activity of the industrial reference at 220 °C.
Mn/TiO2 and Mn–Fe/TiO2 catalysts synthesized by deposition precipitation—promising for selective catalytic reduction of NO with NH3 at low temperatures.

Mn/TiO2 and Mn–Fe/TiO2 catalysts have been prepared by impregnation (IMP) and deposition-precipitation (DP) techniques and characterized by N2 physisorption, XRPD, NH3-TPD, H2-TPR, XPS and TGA. 25 wt% Mn0.75Fe0.25Ti-DP catalyst, prepared by deposition precipitation with ammonium carbamate (AC) as a precipitating agent, showed superior low-temperature SCR (selective catalytic reduction) of NO with NH3. The superior catalytic activity of the 25 wt% Mn0.75Fe0.25Ti-DP catalyst is probably due to the presence of amorphous phases of manganese oxide, iron oxide, high surface area, high total acidity, acid strength and ease of reduction of manganese oxide and iron oxide on TiO2 in addition to formation of an SCR active MnOx phase with high content of chemisorbed oxygen (Oα). The optimum catalyst might be used as tail-end SCR catalysts in, e.g., biomass-fired power plants and waste incineration plants.

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Modeling the Aggregation Propensity and Toxicity of Amyloid-β Variants

Protein aggregation is a hallmark of many neurodegenerative disorders. Alzheimer’s disease (AD) is directly linked to deposits of amyloid-β (Aβ) derived from the amyloid-β protein precursor (AβPP), and multiple experimental studies have investigated the aggregation behavior of these amyloids. The present paper reports modeling of the aggregation propensities and cell toxicities of genetic variants of Aβ known to increase disease risk. From correlation to experimental data, and using four distinct experimental structures to test structural sensitivity, we find that the Spatial Aggregation Propensity (SAP) formalism can describe the relative experimental aggregation propensities of Aβ 42 variants (R2=0.49 and 0.70, p∼0.02 and 0.002, for 1IYT and 1Z0Q conformations using a probe radius of 10Å). Our analysis finds correlation between the reduction in hydrophilic surface and experimental aggregation propensities. Finally, we show that experimental cell toxicities of Aβ variants are well described by computed SAP values, suggesting direct interplay between aggregation propensity and cell toxicity and providing a step toward a first computational estimator of Aβ toxicity. The present study contributes to our understanding of amyloid aggregation and suggests a method to predict aggregation propensity and toxicity of Aβ variants, and potentially to reduce aggregation propensities of amyloids by molecular intervention directed toward specific conformations of the peptides.

General information
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Scopus rating (2012): SJR 1.694 SNIP 1.055 CiteScore 4.35
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BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.525 SNIP 0.906 CiteScore 3.97
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Scopus rating (2009): SJR 1.727 SNIP 1.022
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Scopus rating (2008): SJR 1.545 SNIP 0.963
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Scopus rating (2002): SJR 0.603 SNIP 0.216
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Modeling the liquid-liquid equilibrium of petroleum fluid and polar compounds containing systems with the PC-SAFT equation of state

A critical test for the perturbed-chain statistical associating fluid theory (PC-SAFT) equation of state (EOS) is the modeling of systems containing petroleum fluid and polar compounds. In this work, two approaches are proposed for the simplified PC-SAFT EOS to obtain the necessary pure component parameters for the characterized non-associating pseudo-components of petroleum fluids. New pure component parameters of mono-ethylene glycol (MEG) are obtained by considering the liquid liquid equilibrium (LLE) data of MEG with normal hydrocarbons in the estimation process and a simple binary interaction scheme of MEG with pseudo-components is proposed. These new parameters are applied to model LLE of the systems of petroleum fluid + MEG with or without water. The results show that the simplified PC-SAFT EOS yields promising predictions of the key mutual solubility of these systems: 15-18% overall deviations for the systems of petroleum fluid + MEG and 23-25% overall deviations for the systems of petroleum fluid + MEG + water. The two approaches are further studied in a more theoretical manner to show the relationship between the solubility of petroleum fluid in the polar phase and the PC-SAFT parameter segment diameter. (C) 2015 Elsevier B.V. All rights reserved.
Molybdenum-catalyzed conversion of diols and biomass-derived polyols to alkenes using isopropyl alcohol as reductant and solvent

Chemical processes capable of reducing the high oxygen content of biomass-derived polyols are in demand in order to produce renewable substitutes for chemicals of fossil origin. Deoxydehydration (DODH) is an attractive reaction that in a single step transforms a vicinal diol into an alkene, but the reaction requires a homogeneous catalyst, a reductant, and a solvent, which are typically expensive, unsustainable, or inefficient. Herein, we present the use of molybdenum(VI)-based compounds, in particular the cheap and commercially available (NH₄)₆Mo₇O₂₄·4H₂O, as catalysts for the DODH of vicinal diols in isopropyl alcohol (iPrOH), which serves as both the solvent and reductant. The reaction proceeds at 240-250 °C in a pressurized autoclave, and the alkene yield from simple aliphatic diols can be as high as 77%. The major byproducts are carbonyl compounds - formed by dehydration of the diol - and the alcohols formed by transfer hydrogenation of the carbonyl compounds; the total yield of reduced species (i.e., alkene and alcohols) can be as high as 92%. The DODH of glycerol yields allyl alcohol, which undergoes subsequent Mo-catalyzed deoxygenation to propylene driven by the oxidation of iPrOH; a major byproduct is the homo-coupled product 1,5-hexadiene. Further insight in this Mo-catalyzed deoxygenation is gained by an investigation of model compounds: The allylic alcohol 1-hexen-3-ol is deoxygenated to hexene isomers in a yield of 65%, while benzyl alcohol is deoxygenated to toluene in a yield of 93%. The DODH of erythritol yields 39% 2,5-dihydrofuran, while the DODH of the proposed intermediate 1,4-anhydroerythritol yields 75%. The mechanism of the DODH of 1,4-anhydroerythritol was investigated by means of density functional theory (DFT), and the rate-determining step (24.1 kcal/mol) was found to be reduction of a molybdenum(VI) diolate to a molybdenum(IV) diolate.

General information
State: Published
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Monocyte targeting and activation by cationic liposomes formulated with a TLR7 agonist

Objectives: Monocytes are one of the major phagocytic cells that patrol for invading pathogens, and upon activation, differentiate into macrophages or antigen-presenting dendritic cells (DCs) capable of migrating to lymph nodes eliciting an adaptive immune response. The key role in regulating adaptive immune responses has drawn attention to modulate monocyte responses therapeutically within cancer, inflammation and infectious diseases. We present a technology for targeting of monocytes and delivery of a toll-like receptor (TLR) agonist in fresh blood using liposomes with a positively charged surface chemistry.

Methods: Liposomes were extruded at 100 nm, incubated with fresh blood, followed by leukocyte analyses by FACS. Liposomes with and without the TLR7 agonist TMX-202 were incubated with fresh blood, and monocyte activation measured by cytokine secretion by ELISA and CD14 and DC-SIGN expression.

Results: The liposomes target monocytes specifically over lymphocytes and granulocytes in human whole blood, and show association with 75 - 95% of the monocytes after 1 h incubation. Formulations of TMX-202 in cationic liposomes were potent in targeting and activation of monocytes, with strong induction of IL-6 and IL-12p40, and differentiation into CD14+ and DC-SIGN+ DCs.

Conclusion: Our present liposomes selectively target monocytes in fresh blood, enabling delivery of TLR7 agonists to the intracellular TLR7 receptor, with subsequent monocyte activation and boost in secretion of proinflammatory cytokines. We envision this technology as a promising tool in future cancer immunotherapy.
Multicomponent Adsorption Model for Polar and Associating Mixtures

The multicomponent potential adsorption theory (MPTA) is revisited in this work for polar and associating systems. MPTA is used in combination with the CPA equation of state. Previous studies have shown that both MPTA and other theories present difficulties for complex systems. Some of these problems could be due to the fact that the original MPTA assumes that a given adsorbent has the same adsorption capacity (for example, porous volume) for all the adsorbed substances and is adjusted simultaneously to many data. This is a simplified picture, as experimental data indicate that the adsorption capacities of the various components may also differ. In this paper, we develop a scheme for the distribution of the potential, which accounts for the presence of the porous space occupied either by just one component or by both components. These capacities are determined by adjustment of the potentials to experimental data on single-component adsorption. We show that MPTA involving the different adsorption capacities for the different components is capable of predicting binary adsorption data for most of the mixtures considered. In our application of MPTA, we used both the well-
known Dubinin-Radushkevich-Astakhov potentials and the potentials directly restored from experimental data by solving
the inverse problem. Application of the latter potentials clearly demonstrates the importance of the difference in adsorption
capacities. However, the quality of prediction of binary adsorption is similar for both potentials. Thus, we feel that there is
no need to use more complex potentials provided that the difference in the individual adsorption capacities is accounted
for.

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Organisations: Center for Energy Resources Engineering, Department of Chemistry, Physical and Biophysical Chemistry,
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Scopus rating (2014): SJR 1.012 SNIP 1.292 CiteScore 2.85
Web of Science (2014): Indexed yes
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Scopus rating (2013): SJR 0.982 SNIP 1.243 CiteScore 2.6
ISI indexed (2013): ISI indexed yes
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Scopus rating (2009): SJR 1.002 SNIP 1.164
Web of Science (2009): Indexed yes
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Scopus rating (2008): SJR 1.142 SNIP 1.267
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Multi-function anti-fouling bio-active surfaces

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Multiple diguanylate cyclase-coordinated regulation of pyoverdine synthesis in Pseudomonas aeruginosa

The nucleotide signalling molecule bis-(3'-5')-cyclic dimeric guanosine monophosphate (c-di-GMP) plays an essential role in regulating microbial virulence and biofilm formation. C-di-GMP is synthesized by diguanylate cyclase (DGC) enzymes and degraded by phosphodiesterase (PDE) enzymes. One intrinsic feature of c-di-GMP signalling is the abundance of DGCs and PDEs encoded by many bacterial species. It is unclear whether the different DGCs or PDEs coordinately establish the c-di-GMP regulation or function independently of each other. Here, we provide evidence that multiple DGCs are involved in regulation of c-di-GMP on synthesis of the major iron siderophore pyoverdine in Pseudomonas aeruginosa.

Constitutive expression of the WspG or YedQ DGC in P.aeruginosa is able to induce its pyoverdine synthesis. Induction of pyoverdine synthesis by high intracellular c-di-GMP depends on the synthesis of exopolysaccharides and another two DGCs, SiaD and SadC. SiaD was found to boost the c-di-GMP synthesis together with constitutively expressing YedQ. The exopolysaccharides and the SiaD DGC were found to modulate the expression of the RsmY/RsmZ ncRNAs. Induction of the RsmY/RsmZ ncRNAs might enhance the pyoverdine synthesis through SadC. Our study sheds light on a novel multiple DGC-coordinated c-di-GMP regulatory mechanism of bacteria.

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Scopus rating (2013): SJR 1.465 SNIP 0.941 CiteScore 3.24
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Mussel-inspired bio functionalization of graphene for electrochemical sensor applications

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Mutants of *Micromonospora viridifaciens* sialidase have highly variable activities on natural and non-natural substrates

This study aimed to improve the hydrolase activity of the well-characterised bacterial sialidase from *Micromonospora viridifaciens*. The enzyme and its mutated versions were produced in *Bacillus subtilis* and secreted to the growth medium. Twenty amino acid positions in or near the active site were subjected to site-saturation mutagenesis and evaluated on the artificial sialidase substrate 2-O-(p-nitrophenyl)-α-d-N-acetyleneuraminic acid and on the natural substrate casein glycomacropeptide. A considerably higher fraction of the mutants exhibited increased activity on the artificial substrate compared with the natural one, with the most proficient mutant showing a 13-fold improvement in $k_{cat}/K_m$. In contrast, no mutants displayed more than a 2-fold increase in activity on the natural substrate. To gain further insight into this important discrepancy, we analysed the stability of mutants using the PoPMuSiC software, a property that also correlates with the potential for introducing chemical variation, after validating the method with a set of experimental stability estimates. We found a significant correlation between improved hydrolase activity on the artificial substrate and reduced apparent stability. Together with the minor improvement on the natural substrate this shows an important difference between naturally evolved functionality and new laboratory functionality. Our results suggest that when engineering sialidases and potentially other proteins towards non-natural substrates that are not optimized by natural evolution, major changes in chemical properties are advantageous, and these changes tend to correlate with decreased stability, partly explaining commonly observed trade-offs between stability and proficiency.
Mutational analysis of divalent metal ion binding in the active site of class II α-mannosidase from Sulfolobus solfataricus

Mutational analysis of Sulfolobus solfataricus class II α-mannosidase was focused on side chains that interact with the hydroxyls of the-1 mannosyl of the substrate (Asp-534) or form ligands to the active site divalent metal ion (His-228 and His-533) judged from crystal structures of homologous enzymes. D534A and D534N appeared to be completely inactive. When compared to the wild-type enzyme, the mutant enzymes in general showed only small changes in KM for the substrate, p-nitrophenyl-α-mannoside, but elevated activation constants, KA, for the divalent metal ion (Co2+, Zn2+, Mn2+, or Cd2+). Some mutant enzyme forms displayed an altered preference for the metal ion compared to that of the wild type-enzyme. Furthermore, the H228Q, H533E, and H533Q enzymes were inhibited at increasing Zn2+ concentrations. The catalytic rate was reduced for all enzymes compared to that of the wild-type enzyme, although less dramatically with some activating metal ions. No major differences in the pH dependence between wild-type and mutant enzymes were found in the presence of different metal ions. The pH optimum was 5, but enzyme instability was observed at pH

General information
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NMR Insights into the Inner Workings of Living Cells

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BFI (2018): BFI-level 2
Oligomerization of a Glucagon-like Peptide 1 Analog: Bridging Experiment and Simulations

The glucagon-like peptide 1 (GLP-1) analog, liraglutide, is a GLP-1 agonist and is used in the treatment of type-2 diabetes mellitus and obesity. From a pharmaceutical perspective, it is important to know the oligomerization state of liraglutide with respect to stability. Compared to GLP-1, liraglutide has an added fatty acid (FA) moiety that causes oligomerization of liraglutide as suggested by small-angle x-ray scattering (SAXS) and multiangle static light scattering (MALS) results. SAXS data suggested a global shape of a hollow elliptical cylinder of size hexa-, hepta-, or octamer, whereas MALS data indicate a hexamer. To elaborate further on the stability of these oligomers and the role of the FA chains, a series of molecular-dynamics simulations were carried out on 11 different hexa-, hepta-, and octameric systems. Our results indicate that interactions of the fatty acid chains contribute noticeably to the stabilization. The simulation results indicate that the heptamer with paired FA chains is the most stable oligomer when compared to the 10 other investigated structures. Theoretical SAXS curves extracted from the simulations qualitatively agree with the experimentally determined SAXS curves supporting the view that liraglutide forms heptamers in solution. In agreement with the SAXS data, the heptamer forms a water-filled oligomer of elliptical cylindrical shape.
One-step Facile Functionalization of Graphene for Highly Active Electrocatalysis

General information
State: Published
Organisations: Department of Chemistry, NanoChemistry, Organic Chemistry
Authors: Zhang, M. (Intern), Ulstrup, J. (Intern), Chi, Q. (Intern)
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On the calculation of x-ray scattering signals from pairwise radial distribution functions
We derive a formulation for evaluating (time-resolved) x-ray scattering signals of solvated chemical systems, based on pairwise radial distribution functions, with the aim of this formulation to accompany molecular dynamics simulations. The derivation is described in detail to eliminate any possible ambiguities, and the result includes a modification to the atom-type formulation which to our knowledge is previously unaccounted for. The formulation is numerically implemented and validated.

General information
State: Published
Organisations: Center for Atomic-scale Materials Design, Department of Chemistry, Department of Physics, Neutrons and X-rays for Materials Physics, Physical and Biophysical Chemistry
Authors: Dohn, A. O. (Intern), Biasin, E. (Intern), Haldrup, K. (Intern), Nielsen, M. M. (Intern), Henriksen, N. E. (Intern), Møller, K. B. (Intern)
Number of pages: 9
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Main Research Area: Technical/natural sciences

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Journal: Journal of Physics B: Atomic, Molecular and Optical Physics
Volume: 48
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Article number: 244010
ISSN (Print): 0953-4075
Ratings:
BFI (2018): BFI-level 2
On the viscosity of two 1-butyl-1-methylpyrrolidinium ionic liquids: effect of the temperature and pressure

A new calibration procedure was used and four new temperature probes have been placed on a falling-body viscometer to improve its accuracy. The new configuration and calibration procedure allow measuring viscosities with an uncertainty of 3.5% at pressures up to 150 MPa. This device was employed to measure viscosities as a function of temperature and...
pressure for two ionic liquids (ILs): 1-butyl-1-methylpyrrolidinium
tris(pentafluoroethyl)trifluorophosphate and 1-butyl-1-methylpyrrolidinium trifluoromethanesulfonate. Besides, we have
measured the flow curves at pressures up to 75 MPa and shear rates up to 1000 s⁻¹ in a Couette rheometer. Dynamic
viscosities were correlated as function of temperature and pressure with four different equations with average absolute
deviation lower than 1%. The pressure-viscosity and temperature-viscosity derived properties were analyzed and
compared with those of other ionic liquids. Furthermore, experimental data were used to check the application of the
thermodynamic scaling approach as well as the hard-sphere scheme. Both models represent the viscosity values with
average relative deviations lower than 2%.

General information
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Organisations: Center for Energy Resources Engineering, Department of Chemistry, Department of Chemical and
Biochemical Engineering, CERE – Center for Energy Resources Engineering, University of Santiago de Compostela,
University of Valladolid, Universidad de Santiago de Compostela
Authors: Gaciño, F. M. (Ekstern), Comuñas, M. J. (Ekstern), Regueira Muñiz, T. (Intern), Segovia, J. J. (Ekstern),
Fernández, J. (Ekstern)
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.64 SJR 1 SNIP 1.163
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.075 SNIP 1.091 CiteScore 2.29
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.224 SNIP 1.306 CiteScore 2.59
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.252 SNIP 1.25 CiteScore 2.42
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.221 SNIP 1.181 CiteScore 2.41
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Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.24 SNIP 1.307 CiteScore 2.44
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.218 SNIP 1.462
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.116 SNIP 1.355
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.414 SNIP 1.269
Scopus rating (2007): SJR 1.264 SNIP 1.176
Optimization of anti-cobratoxins for treatment of neurotoxic envenomings

Cobras (Naja spp.) are some of the most venomous and dangerous snakes worldwide, responsible for high mortality and morbidity. The most toxic components of cobra venoms are cobratoxins, which target the nicotinic acetylcholine receptors (nAChRs) responsible for neuromuscular transmission. Inhibition of nAChRs may lead to respiratory arrest with death as a result within 3-12 hr after a bite from a cobra. Early parental administration of appropriate antivenom is the cornerstone of life saving snakebite therapy. However, current antivenoms are still produced by animal immunization, which is a laborious and expensive process yielding highly immunogenic antivenoms due to the heterologous nature of equine antibodies in the antivenom. In contrast, novel antivenom based on synthetic peptides may offer an alternative solution, which is less expensive and cause less side effects.

Oxidative Umpolung α-Alkylation of Ketones

We disclose a hypervalent iodine mediated α-alkylative umpolung reaction of carbonyl compounds with dialkylzinc as the alkyl source. The reaction is applicable to all common classes of ketones including 1,3-dicarbonyl compounds and regular ketones via their lithium enolates. The α-alkylated carbonyl products are formed in up to 93% yield. An ionic mechanism is inferred based on meticulous analysis, NMR studies, trapping and crossover experiments, and computational studies.
Oxygen Sorption and Desorption Properties of Selected Lanthanum Manganites and Lanthanum Ferrite Manganites

Temperature-programmed desorption (TPD) with a carrier gas was used to study the oxygen sorption and desorption properties of oxidation catalysts and solid-oxide fuel cell (SOFC) cathode materials (La$_{0.85}$Sr$_{0.15}$O$_{1.95}$MnO$_{3+\delta}$ (LSM) and La$_{0.60}$Sr$_{0.40}$Fe$_{0.80}$Mn$_{0.20}$O$_{3-\delta}$ (LSFM)). The powders were characterized by X-ray diffractometry, atomic force microscopy (AFM), and BET surface adsorption. Sorbed oxygen could be distinguished from oxygen originating from stoichiometry changes. The results indicated that there is one main site for oxygen sorption/desorption. The amount of sorbed oxygen was monitored over time at different temperatures. Furthermore, through data analysis it was shown that the desorption peak associated with oxygen sorption is described well by second-order desorption kinetics. This indicates that oxygen molecules dissociate upon adsorption and that the rate-determining step for the desorption reaction is a recombination of monatomic oxygen. Typical problems with re-adsorption in this kind of TPD setup were revealed to be insignificant by using simulations. Finally, different key parameters of sorption and desorption were determined, such as desorption activation energies, density of sorption sites, and adsorption and desorption reaction order.
Pathogenic properties of Alzheimer’s β-amyloid identified from structure–property patient-phenotype correlations. β-Amyloid (Aβ) plays a central role in Alzheimer’s disease (AD), but the specific molecular mechanism and associated structures remain unknown. We compiled patient data for carriers of genetic variants of Aβ that cause AD and correlated these data against chemical properties for 56 mutant conformations derived from four published experimental conformations of Aβ of variable structure and chemical environment. Disease onset of variants is significantly (p<0.006) correlated to hydrophobic surfaces of disordered conformations (2LFM), whereas structured conformations yielded no correlations. Correlation also applied (p<0.03) to in vitro steady-state Aβ levels. We conclude that disordered monomers are likely to be pathogenically important in contrast to structured conformations and that hydrophobic surface correlates with pathogenesis. This first established correlation between clinical and chemical data suggests that specific exposed, disordered monomers are viable targets for AD therapy.

General information
State: Published
Organisations: Department of Chemistry, Physical and Biophysical Chemistry
Authors: Tiwari, M. K. (Intern), Kepp, K. P. (Intern)
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Web of Science (2018): Indexed yes
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Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Reservoir fluids are multicomponent mixtures in confined spaces, where the role of capillary force becomes important when the average pore size is on the order of tens of nanometers, such as in tight rocks and shale. We present an algorithm for calculating the phase envelope of multicomponent mixtures in the presence of capillary pressure. The algorithm uses a rigorous equation of state (EoS) model, such as the Soave-Redlich-Kwong EoS, for phase equilibrium, and the Young-Laplace equation for the capillary pressure. The interfacial tension is calculated using a parachor based model. A full Newton method is employed to solve the governing equations of the vapor-liquid equilibria coupled with the capillary pressure equation. For a stable and automatic construction of the phase envelope sensitivity analysis is used in...
each step. The developed algorithm can reliably generate not just the bubble and dew point curves but also other quality lines with vapor fractions between 0 and 1. The algorithm has been used to calculate the phase envelopes of binary, multicomponent and reservoir fluid systems for pore radius from 10 to 50 nm. The presence of capillary pressure changes the saturation pressures in the whole phase envelope except at the critical point. The bubble point curve shows a negative change while the dew point curve shows positive and negative changes in the upper dew point branch and the lower dew point branch, respectively. In particular, the cricondentherm is also shifted towards a higher temperature. The change in the phase envelope becomes larger as the pore size decreases. The effects of composition and gas oil ratios are also discussed.

Porous poly(perfluorosulfonic acid) membranes for alkaline water electrolysis

Poly(perfluorosulfonic acid) (PFSA) is one of a few polymer types that combine excellent alkali resistance with extreme hydrophilicity. It is therefore of interest as a base material in separators for alkaline water electrolyzers. In the pristine form it, however, shows high cation selectivity. To increase its ion conductivity in aqueous KOH, a method for the preparation of porous PFSA membranes was developed. It was based on an approach where PFSA was co-cast with poly(vinylpyrrolidone) (PVP) at different ratios to give transparent and colorless blend membranes. The PVP was subsequently dissolved and washed out and the obtained porous materials allowed for swelling to reach water contents up to λ=85 [H₂O] [−SO₃K]−1. After equilibration in 22 wt% aqueous KOH, ion conductivity of 0.2 S cm⁻¹ was recorded for this membrane type at room temperature, which is significantly higher than 0.01 S cm⁻¹ for the unmodified membrane. The technological feasibility was demonstrated by testing the membranes in an alkaline water electrolysis cell with encouraging performance.
Since the first report of the enhanced permeability and retention (EPR) effect, the research in nanocarrier based antitumor drugs has been intense. The field has been devoted to treatment of cancer by exploiting EPR-based accumulation of nanocarriers in solid tumors, which for many years was considered to be a ubiquitous phenomenon. However, the understanding of differences in the EPR-effect between tumor types, heterogeneities within each patient group, and dependency on tumor development stage in humans is sparse. It is therefore important to enhance our understanding of the EPR-effect in large animals and humans with spontaneously developed cancer. In the present paper, we describe a novel loading method of copper-64 into PEGylated liposomes and use these liposomes to evaluate the EPR-effect in 11 canine cancer patients with spontaneous solid tumors by PET/CT imaging. We thereby provide the first high-resolution
analysis of EPR-based tumor accumulation in large animals. We find that the EPR-effect is strong in some tumor types but cannot be considered a general feature of solid malignant tumors since we observed a high degree of accumulation heterogeneity between tumors. Six of seven included carcinomas displayed high uptake levels of liposomes, whereas one of four sarcomas displayed signs of liposome retention. We conclude that nanocarrier-radiotracers could be important in identifying cancer patients that will benefit from nanocarrier-based therapeutics in clinical practice.
Pressure dependence of the solubility of light fullerenes in 1-hexanol from 298.15 K to 363.15 K

The solubility of light fullerenes (C\textsubscript{60} and C\textsubscript{70}) in 1-hexanol was investigated in the range of pressures of 0.1-100 MPa and in the range of temperatures of 298.15-363.15 K. In all of the studied temperatures, solubility increases monotonously with increasing pressure. At ambient pressure, we have found that the temperature dependence of solubility in the binary system C\textsubscript{60}-1-hexanol is non-monotonic: the solubility diagram consists of two branches corresponding to the crystallization of different solid phases and one invariant point corresponding to the simultaneous saturation of both phases (monosolvated fullerene C\textsubscript{60} and non-solvated C\textsubscript{60}). The composition of the solid crystallosolvate was determined by thermogravimetric analysis. The solubility diagram of the binary system C\textsubscript{70}-1-hexanol in the temperature range of 298.15-328.15 K at 0.1 MPa consists of only one branch corresponding to the crystallization of non-solvated C\textsubscript{70}.

General information

State: Published
Organisations: Center for Energy Resources Engineering, Department of Chemistry, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, St. Petersburg State University, Universidad de Santiago de Compostela
Authors: Semenov, K. N. (Ekstern), Regueira Muñiz, T. (Intern), Fernández, J. (Ekstern), Charykov, N. A. (Ekstern), Murin, I. V. (Ekstern)
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BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.47 SJR 0.718 SNIP 1.212
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.652 SNIP 0.997 CiteScore 2.61
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.637 SNIP 1.126 CiteScore 2.34
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.611 SNIP 1.082 CiteScore 2.07
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.673 SNIP 1.041 CiteScore 1.62
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.611 SNIP 1.093 CiteScore 1.64
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.691 SNIP 1.139
Probing Bio-Nano Interactions between Blood Proteins and Monolayer-Stabilized Graphene Sheets

Meeting proteins is regarded as the starting event for nanostructures to enter biological systems. Understanding their interactions is thus essential for a newly emerging field, nanomedicine. Chemically converted graphene (CCG) is a wonderful two-dimensional (2D) material for nanomedicine, but its stability in biological environments is limited. Systematic probing on the binding of proteins to CCG is currently lacking. Herein, we report a comprehensive study on the interactions between blood proteins and stabilized CCG (sCCG). CCG nanosheets are functionalized by monolayers of perylene leading to significant improvement in their resistance to electrolyte salts and long-term stability, but retain their core structural characteristics. Five types of model human blood proteins including human fibrinogen, γ-globulin, bovine serum albumin (BSA), insulin, and histone are tested. The main driving forces for blood protein binding involve the π–π interactions between the π-plane of sCCG and surface aromatic amonic acid (sAA) residues of proteins. Several key binding parameters including the binding amount, Hill coefficient, and binding constant are determined. Through a detailed analysis of key controlling factors, we conclude that the protein binding to sCCG is determined mainly by the protein size, the number, and the density of the sAA.

General information
State: Published
Organisations: NanoChemistry, Department of Chemistry, Chinese Academy of Sciences
Authors: Gan, S. (Intern), Zhong, L. (Ekstern), Han, D. (Ekstern), Niu, L. (Ekstern), Chi, Q. (Intern)
Number of pages: 12
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BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 8.11 SJR 3.324 SNIP 1.505
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Process for the conversion of sugars to lactic acid and 2-hydroxy-3-butenoic acid or esters thereof comprising a metallosilicate material and a metal ion

A process for the preparation of lactic acid and 2-hydroxy-3-butenoic acid or esters thereof from a sugar in the presence of a metallosilicate material, a metal ion and a solvent, wherein the metal ion is selected from one or more of the group consisting of potassium ions, sodium ions, lithium ions, rubidium ions and caesium ions.

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry, Haldor Topsoe AS
Authors: Holm, M. S. (Ekstern), Irantzú, S. Z. (Ekstern), Tolborg, S. (Intern), Osmundsen, C. M. (Intern), Taarning, E. (Ekstern)
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PVT modeling of reservoir fluids using PC-SAFT EoS and Soave-BWR EoS

Cubic equations of state, such as the Soave-Redlich-Kwong (SRK) and the Peng-Robinson (PR) EoS, are still the mostly used models in PVT modeling of reservoir fluids, and almost the exclusively used models in compositional reservoir simulations. Nevertheless, it is promising that recently developed non-cubic EoS models, such as the Perturbed Chain Statistical Associating Fluid Theory (PC-SAFT) EoS and the Soave modified Benedict-Webb-Rubin (Soave-BWR) EoS, may partly replace the roles of these classical cubic models in the upstream oil industry. Here, we attempt to make a comparative study of non-cubic models (PC-SAFT and Soave-BWR) and cubic models (SRK and PR) in several important aspects related to PVT modeling of reservoir fluids, including density description for typical pure components in reservoir fluids, description of binary VLE, prediction of multicomponent phase envelopes, and PVT calculation of reservoir fluids. Extensive data are used in the comparison and the four models are treated as equally as possible. We adopt the method of Pedersen et al. as the framework for heptanes plus characterization and the same correlations for estimating the critical properties for SRK, PR and Soave-BWR. For PC-SAFT, new correlations for estimating its model parameters in heptanes plus are developed. The results reveal that the non-cubic models are clearly advantageous in density calculation of pure components. For binary VLE and multicomponent phase envelopes, the results are similar for the four models. For PVT prediction, the non-cubic models show advantages in some high pressure high temperature (HPHT) fluids but no clear advantages in general, indicating the necessity for further improvement of the characterization procedure.
Pyrazole Based Inhibitors against Enzymes of Staphylococcus aureus: A Computational Study

Pyrazole derivatives display a wide variety of biological activities such as antimicrobial, anti-inflammatory and anti-tumor activities. Its biological prominence has intrigued chemists and biologists in recent years to synthesize new pyrazole derivatives as antiviral, antibacterial and anticancer agents. The current study focuses on molecular docking and dynamics studies of pyrazole derivatives against Nucleosidase and DNA gyrase B of Staphylococcus aureus. Molecular docking and dynamics studies reveal that some of these derivatives show better binding abilities than some of the current drugs available on the market.

General information
State: Published
Organisations: Department of Chemistry, University of Madras, Presidency College, Chennai, Roskilde University
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Volume: 8
Reductive Cyclization and Petasis-Like Reaction for the Synthesis of Functionalized γ-Lactams

An efficient reductive cyclization strategy was employed for the synthesis of N-substituted β,γ-dihydroxy-γ-lactams. A subsequent Petasis-like reaction (PLR) through nucleophilic additions of boronic acids to intermediate N-acyliminium ions produced substituted γ-lactams. Overall, the application of this protocol provides β,γ-dihydroxy-γ-lactams and functionalized γ-lactams with potential interest for synthetic and bioorganic chemistry.

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry, Center for Nanomedicine and Theranostics
Authors: Wu, P. (Intern), Petersen, M. Á. (Intern), Cohrt, A. E. (Intern), Petersen, R. (Intern), Clausen, M. H. (Intern), Nielsen, T. E. (Intern)
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Scopus rating (2016): CiteScore 2.74 SJR 1.133 SNIP 0.653
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.198 SNIP 0.758 CiteScore 2.88
Web of Science (2015): Indexed yes
Remote Loading of $^{64}$Cu$^{2+}$ into Liposomes without the Use of Ion Transport Enhancers

Due to low ion permeability of lipid bilayers, it has been and still is common practice to use transporter molecules such as ionophores or lipophilic chelators to increase transmembrane diffusion rates and loading efficiencies of radionuclides into liposomes. Here, we report a novel and very simple method for loading the positron emitter $^{64}$Cu$^{2+}$ into liposomes, which is important for in vivo positron emission tomography (PET) imaging. By this approach, copper is added to liposomes entrapping a chelator, which causes spontaneous diffusion of copper across the lipid bilayer where it is trapped. Using this method, we achieve highly efficient $^{64}$Cu$^{2+}$ loading (>95%), high radionuclide retention (>95%), and favorable loading kinetics, excluding the use of transporter molecule additives. Therefore, clinically relevant activities of 200-400 MBq/patient can be loaded fast (60-75 min) and efficiently into preformed stealth liposomes avoiding subsequent
purification steps. We investigate the molecular coordination of entrapped copper using X-ray absorption spectroscopy and demonstrate high adaptability of the loading method to pegylated, nonpegylated, gel- or fluid-like, cholesterol rich or cholesterol depleted, cationic, anionic, and zwitterionic lipid compositions. We demonstrate high in vivo stability of $^{64}$Cu-liposomes in a large canine model observing a blood circulation half-life of 24 h and show a tumor accumulation of 6% ID/g in FaDu xenograft mice using PET imaging. With this work, it is demonstrated that copper ions are capable of crossing a lipid membrane unassisted. This method is highly valuable for characterizing the in vivo performance of liposome-based nanomedicine with great potential in diagnostic imaging applications.
Resolution and Determination of the Absolute Configuration of a Twisted Bis-Lactam Analogue of Troger's Base: A Comparative Spectroscopic and Computational Study

The first reported twisted bis-lactam, a racemic Troger's base (TB) analogue (2), was resolved into its enantiomers on a chiral stationary phase HPLC column. The absolute configuration of (+)-2 was determined to be (R,R)-2 by comparing experimental and calculated vibrational circular dichroism (VCD) and electronic circular dichroism (ECD) spectra. The absolute configuration of (-)-2 was determined by comparing experimental and calculated electronic circular dichroism (ECD) spectra. The corresponding theoretical spectra were calculated using the lowest energy conformation of (R,R)-2 and (S,S)-2 at the B3LYP/6-31G(d,p) level of theory. The absolute configuration of (+)-2 was also determined to (R,R)-2 by anomalous X-ray diffraction (AXRD) in a chiral space group P2(1)2(1)2(1) using Cu-irradiation resulting in a very low Flack parameter of -0.06(3), despite the heaviest element being an oxygen atom, thus unambiguously confirming the results from the spectroscopic studies. We conclude that, for the Troger's base (TB) analogue (2), we may rank the reliability of the individual methods for AC determination as AXRD >> VCD > ECD, while the synergy of all three methods provides very strong confidence in the assigned ACs of (+)-(R,R)-2 and (-)-(S,S)-2.

General information
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Organisations: Department of Chemistry, Organic Chemistry, Lund University, University of Bonn, University of Missouri, Queen's University, University of Jyväskyla
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Scopus rating (2016): CiteScore 4.59 SJR 1.976 SNIP 1.03
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 2.018 SNIP 1.174 CiteScore 4.69
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Scopus rating (2014): SJR 2.003 SNIP 1.222 CiteScore 4.69
Web of Science (2014): Indexed yes
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Scopus rating (2013): SJR 2.078 SNIP 1.176 CiteScore 4.51
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 2.272 SNIP 1.23 CiteScore 4.31
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Rhenium-Catalyzed Deoxydehydration of Diols and Polyols

The substitution of platform chemicals of fossil origin by biomass-derived analogues requires the development of chemical transformations capable of reducing the very high oxygen content of biomass. One such reaction, which has received increasing attention within the past five years, is the rhenium-catalyzed deoxydehydration (DODH) of a vicinal diol into an alkene; this is a model system for abundant polyols like glycerol and sugar alcohols. The present contribution includes a review of early investigations of stoichiometric reactions involving rhenium, diols, and alkenes followed by a discussion of the various catalytic systems that have been developed with emphasis on the nature of the reductant, the substrate scope, and mechanistic investigations.

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry
Authors: Dethlefsen, J. R. (Intern), Fristrup, P. (Intern)
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Main Research Area: Technical/natural sciences

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ISSN (Print): 1864-5631
Ritter-Hydrolysis Cascade Strategy for the Synthesis of Substituted gamma-Lactams

General information
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Organisations: Department of Chemistry, Organic Chemistry
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Sandwiched confinement of quantum dots in graphene matrix for efficient electron transfer and photocurrent production

Quantum dots (QDs) and graphene are both promising materials for the development of new-generation optoelectronic devices. Towards this end, synergic assembly of these two building blocks is a key step but remains a challenge. Here, we show a one-step strategy for organizing QDs in a graphene matrix via interfacial self-assembly, leading to the formation of sandwiched hybrid QD-graphene nanofilms. We have explored structural features, electron transfer kinetics and photocurrent generation capacity of such hybrid nanofilms using a wide variety of advanced techniques. Graphene nanosheets interlink QDs and significantly improve electronic coupling, resulting in fast electron transfer from photoexcited QDs to graphene with a rate constant of $1.3 \times 10^9$ s$^{-1}$. Efficient electron transfer dramatically enhances photocurrent generation in a liquid-junction QD-sensitized solar cell where the hybrid nanofilm acts as a photoanode. We thereby demonstrate a cost-effective method to construct large-area QD-graphene hybrid nanofilms with straightforward scale-up potential for optoelectronic applications.
Seawater as Alternative to Freshwater in Pretreatment of Date Palm Residues for Bioethanol Production in Coastal and/or Arid Areas

The large water consumption (1.9-5.9 m³ water per m³ of biofuel) required by biomass processing plants has become an emerging concern, which is particularly critical in arid/semiarid regions. Seawater, as a widely available water source, could be an interesting option. This work was to study the technical feasibility of using seawater to replace freshwater in the pretreatment of date palm leaflets, a lignocellulosic biomass from arid regions, for bioethanol production. It was shown that leaflets pretreated with seawater exhibited lower cellulose crystallinity than those pretreated with freshwater. Pretreatment with seawater produced comparably digestible and fermentable solids to those obtained with freshwater. Moreover, no significant difference of inhibition to *Saccharomyces cerevisiae* was observed between liquids from pretreatment with seawater and freshwater. The results showed that seawater could be a promising alternative to freshwater for lignocellulose biorefineries in coastal and/or arid/semiarid areas.

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Simultaneous Disulfide and Boronic Acid Ester Exchange in Dynamic Combinatorial Libraries

Dynamic combinatorial chemistry has emerged as a promising tool for the discovery of complex receptors in supramolecular chemistry. At the heart of dynamic combinatorial chemistry are the reversible reactions that enable the exchange of building blocks between library members in dynamic combinatorial libraries (DCLs) ensuring thermodynamic control over the system. If more than one reversible reaction operates in a single dynamic combinatorial library, the complexity of the system increases dramatically, and so does its possible applications. One can imagine two reversible reactions that operate simultaneously or two reversible reactions that operate independently. Both these scenarios have advantages and disadvantages. In this contribution, we show how disulfide exchange and boronic ester transesterification can function simultaneous in dynamic combinatorial libraries under appropriate conditions. We describe the detailed studies necessary to establish suitable reaction conditions and highlight the analytical techniques appropriate to study this type of system.
Single-vesicle detection and analysis of peptide-induced membrane permeabilization

The capability of membrane-active peptides to disrupt phospholipid membranes is often studied by investigating peptide-induced leakage of quenched fluorescent molecules from large unilamellar lipid vesicles. In this article, we explore two fluorescence microscopy-based single-vesicle detection methods as alternatives to the quenching-based assays for studying peptide-induced leakage from large unilamellar lipid vesicles. Specifically, we use fluorescence correlation spectroscopy (FCS) to study the leakage of fluorescent molecules of different sizes from large unilamellar lipid vesicles dispersed in aqueous solution, and we use confocal imaging of surface-immobilized large unilamellar lipid vesicles to investigate whether there are heterogeneities in leakage between individual vesicles. Of importance, we design an experimental protocol that allows us to quantitatively correlate the results of the two methods; accordingly, it can be assumed that the two methods provide complementary information about the same leakage process. We use the two methods to investigate the membrane-permeabilizing activities of three well-studied cationic membrane-active peptides: mastoparan X, melittin, and magainin 2. The FCS results show that leakage induced by magainin 2 is less dependent on the size of the encapsulated fluorescent molecules than leakage induced by mastoparan X and melittin. The confocal
imaging results show that all three peptides induce leakage by a heterogeneous process in which one portion of the vesicles are completely emptied of their contents but another portion of the vesicles are only partially emptied. These pieces of information regarding leakage induced by mastoparan X, melittin, and magainin 2 could not readily have been obtained by the established assays for studying peptide-induced leakage from lipid vesicles.
USER cloning is a fast and versatile method for engineering of plasmid DNA. We have developed a user friendly Web server tool that automates the design of optimal PCR primers for several distinct USER cloning-based applications. Our Web server, named AMUSER (Automated DNA Modifications with USER cloning), facilitates DNA assembly and introduction of virtually any type of site-directed mutagenesis by designing optimal PCR primers for the desired genetic changes. To demonstrate the utility, we designed primers for a simultaneous two-position site-directed mutagenesis of green fluorescent protein (GFP) to yellow fluorescent protein (YFP), which in a single step reaction resulted in a 94% cloning efficiency. AMUSER also supports degenerate nucleotide primers, single insert combinatorial assembly, and flexible parameters for PCR amplification. AMUSER is freely available online at.

Software-Supported USER Cloning Strategies for Site-Directed Mutagenesis and DNA Assembly

USER cloning is a fast and versatile method for engineering of plasmid DNA. We have developed a user friendly Web server tool that automates the design of optimal PCR primers for several distinct USER cloning-based applications. Our Web server, named AMUSER (Automated DNA Modifications with USER cloning), facilitates DNA assembly and introduction of virtually any type of site-directed mutagenesis by designing optimal PCR primers for the desired genetic changes. To demonstrate the utility, we designed primers for a simultaneous two-position site-directed mutagenesis of green fluorescent protein (GFP) to yellow fluorescent protein (YFP), which in a single step reaction resulted in a 94% cloning efficiency. AMUSER also supports degenerate nucleotide primers, single insert combinatorial assembly, and flexible parameters for PCR amplification. AMUSER is freely available online at.

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Solid-Phase Synthesis for the Construction of Biologically Interesting Molecules and the Total Synthesis of Trioxacarcin DC-45-A2

This thesis covers three research projects in addition to a literature survey on solid-phase organic synthesis and photolabile linkers. Synthesis of Doxorubicin Derivatives on Photolabile Solid Support. The synthesis of doxorubicin derivatives on photolabile solid support, compatible with bead-based screening, was investigated. Two different strategies for the synthesis of doxorubicin derivatives were developed leading to the synthesis of doxorubicin derivatives with both amino acids and peptide fragments attached in good to excellent crude purities. Total Synthesis of Trioxacarcin DC-45-A2. In efforts towards the total synthesis of trioxacarcin DC-45-A2 by the Nicolaou group anew and efficient route for a key fragment was optimized. The new route featured distinct and high yielding steps and thus provided superior access to this key building block in terms of overall yield, step count and scalability. Furthermore a route to another key building block was developed featuring a Stille cross-coupling. Synthesis of Poly-fused Heterocycles. In the search for new biologically active compounds a methodology for the synthesis of polyfused heterocycles was investigated. This led to the development and optimization of a key aldol condensation/conjugate addition sequence for the synthesis of poly-fused heterocycles.

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Specific Electrical Conductivity in Molten Potassium Dihydrogen Phosphate KH2PO4 Electrolyte at ~300 °C

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Spectroscopic Characterization of a Monomeric, Cyclopentadienyl-Based Rhenium(V) Dioxo Complex

Mononuclear, coordinatively unsaturated rhenium(V) dioxo species of the type XReO₂ (X = Me, substituted cyclopentadienyl) have long been postulated as intermediates in rhenium-catalyzed deoxydehydration, but their characterization was precluded because of aggregation into dimeric or oligomeric structures. Using the bulky 1,2,4-tri-tert-butylcyclopentadienyl (Cp³ttt) ligand, the rhenium(V) dioxo species (Cp³ttt)ReO₂ could now be observed, in equilibrium with the dimeric form [(Cp³ttt)Re(O)μ-O]₂, and characterized by NMR, IR, and UV-vis spectroscopies, as well as electrospray ionization mass spectrometry. (Cp³ttt)ReO₂ is shown to be the primary product of reduction of the rhenium(VII) complex (Cp³ttt)ReO₃ with PPh₃ and demonstrated to react with ethylene glycol significantly faster than its dimeric counterpart, supporting its role as an intermediate in rhenium-catalyzed deoxydehydration reactions.

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Spectroscopic characterization of a monomeric cyclopentadienyl-based rhenium V dioxo complex.

The far-infrared absorption spectra have been recorded for hydrogen-bonded complexes of water with ethanol embedded in cryogenic neon matrices at 2.8 K. The partial isotopic H/D-substitution of the ethanol subunit enabled by a dual inlet deposition procedure enables the observation and unambiguous assignment of the intermolecular high-frequency out-of-plane and the low-frequency in-plane donor OH librational modes for two different conformations of the mixed binary ethanol/water complex. The resolved donor OH librational bands confirm directly previous experimental evidence that ethanol acts as the O⋯HO hydrogen bond acceptor in the two most stable conformations. In the most stable conformation, the water subunit forces the ethanol molecule into its less stable gauche configuration upon dimerization owing to a cooperative secondary weak O⋯HC hydrogen bond interaction evidenced by a significantly blue-shift of the low-frequency in-plane donor OH librational band origin. The strong correlation between the low-frequency in-plane donor OH librational motion and the secondary intermolecular O⋯HC hydrogen bond is demonstrated by electronic structure calculations. The experimental findings are further supported by CCSD(T)-F12/aug-cc-pVQZ calculations of the conformational energy differences together with second-order vibrational perturbation theory calculations of the large-amplitude donor OH librational band origins.
The structural changes occurring during the interaction between β-lactoglobulin (BLG), the major whey protein, and bovine submaxillary mucin (BSM), a major salivary protein, were studied using high and low field Nuclear Magnetic Resonance (NMR), Dynamic Light Scattering (DLS), and Circular Dichroism (CD) spectroscopy. The zeta potentials of the proteins were also measured to provide information on the role of electrostatic forces in the interaction. The ratio between BLG and BSM was 1:1, and pH was adjusted to 3.0, 5.0 and 7.4 at room temperature. These spectroscopic results suggested that the interaction between BSM and BLG led to a compact aggregation. DLS results of the mixture showed a size distribution which is intermediate between that of BLG (215 nm) and BSM (200 nm). While no particular changes in the secondary structure were observed in either BSM or BLG, a weak tertiary structure, observed in BLG only, was further weakened upon interaction with BSM. High field NMR results for the BSM-BLG mixture indicated that spectral differences were mostly observed for solvent exposed groups, especially the mucin glycan chains, while hydrophobic core residues were less affected. The interaction between the two proteins can thus be concluded to be mostly of hydrophilic origin. Moreover, low field NMR measurements showed a decrease in transverse relaxation times in the mixture compared to the pure BLG and buffer solutions. This is possibly connected to fewer hydrophilic binding sites available in the BLG–BSM mixtures for water–protein interaction after aggregation of the two proteins.
Spinning-out university technologies: a role for students in the commercialization process.

Universities engage in technology commercialization, based on different motivations including the goal of accomplishing sustainable innovation with economic and societal impact and diversifying income streams. The latter objectives are better realized from spinning out successful new companies, which compared to licensing create advantages both for the university and the academic inventor. Although universities generally struggle to successfully commercialize research results as new firms, some universities are much better than others at spinning out companies. The research has not identified a singular formula to increase university spin-outs. A common theme in much of the empirical evidence is that academics/university researchers lack knowledge related to market development which must be supplemented for successful commercialization. This study analyses the role of non-research students in developing knowledge about markets to supplement the knowledge-gaps among academics, which as far as we know have not been widely explored. The analysis is based in the context of a technical university which provides a unique opportunity to explore how students working to fulfill academic requirements can create momentum around a technology to increase its spinout potential. The results show that students working with potential spin-out technologies as class projects are seen as non-threatening which allow them to gather useful market information. This early information can stimulate interest leading to partnership development as well as help to identify advantages and challenges for different applications of a technology.
Spin Propensities of Octahedral Complexes From Density Functional Theory

The fundamental balance between high- and low-spin states of transition metal systems depends on both the metal ion and the ligands surrounding it, as often visualized by the spectrochemical series. Most density functionals do not reproduce this balance, and real spin state propensities depend on orbital pairing and vibrational entropies absent in the spectrochemical series. Thus, we systematically computed the tendency toward high or low spin of “text-book” octahedral metal complexes versus ligand and metal type, using eight density functionals. Dispersion effects were generally <5 kJ/mol, favoring low-spin states. Zero-point energies favored high-spin states up to 33 kJ/mol for strong ligands, but down to a few kilojoules per mole for weak ligands. Vibrational entropy also favored high-spin states up to 40 kJ/mol, most for strong ligands. Jahn–Teller distortion in Co(II) low-spin states, particularly stable d^6 low-spin states, and entropy corrections were consistent with experiment. Entropy and zero-point energy corrections were markedly lower for Co(II) and Mn(III), viz., the differential ligand field stabilization energy, and can only be ignored for weak ligands. The data enable simple assessment of spin state propensities versus ligand and metal type and reveal, e.g., that CN^- is consistently weaker than CO for M(II) but stronger than CO for M(III) and SCN^- and NCS^- change order in M(III) versus M(III) complexes. Contrary to expectation based on the spectrochemical series, Cl^- and Br^- are very close in spin state propensity because the pairing penalty for low spin is smaller in Br^- than in Cl^-<H_2O<SCN^-<NCS^-<NH_3<CN^-<CO, whereas for the M(III) complexes, an approximate order is Br^-<Cl^-<H_2O<SCN^-<NCS^-<NH_3<CO<CN^-.
Strategy for nuclear-magnetic-resonance-based metabolomics of human feces

Metabolomic analyses of fecal material are gaining increasing attention because the gut microbial ecology and activity have an impact on the human phenotype and regulate host metabolism. Sample preparation is a crucial step, and in this study we recommend a methodology for extraction and analysis of fresh feces by NMR-based metabolomics. The evaluation of extraction solvents showed that buffer extraction is a suitable approach to extract metabolic information in feces. So, the effects of weight-to-buffer (Wf:Vb) combinations and the effect of sonication and freeze-thaw cycles on the reproducibility, chemical shift variability, and signal to noise ratio (SNR) of the $^1$H NMR spectra were evaluated. Based on our results, we suggest that fresh fecal extraction with a Wf:Vb ratio of 1:2 may be the optimum choice to determine the overall metabolite composition of feces. In fact, more than 60 metabolites have been assigned in the NMR spectra obtained from the fresh fecal buffer extract, and assignment of the lipophilic signals is also presented. To our knowledge, some of the metabolites are reported here for the very first time employing $^1$H NMR spectroscopy on human fecal extracts.

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Structural Investigation of Sodium Layered Oxides Via in Situ Synchrotron X-Ray Diffraction

Sodium layered oxides with mixed transition metals have received significant attention as positive electrode candidates for sodium-ion batteries due to high reversible capacity. Sodium layered oxides would be more promising candidates than lithium-compounds in terms of high stability of MO2 slabs after extraction of Na induced from larger ionic size of Na. In addition, rich crystal chemistry for sodium layered compounds is available since larger Na+ ion is stable in more spacious prismatic site as compared to Li+ ion. In view of this, the phase transformation of layered compounds during electrochemical reaction is generally considered to be a pivotal feature for understanding the relationship between layered structures and electrochemical properties. Here the structure, phase stability, and electrochemical properties of two kinds of layered oxides, P2 and O3, are investigated through in-situ synchrotron XRD experiments. A capillary Na-based cell is designed to minimize interference in other substances such as a separator or external battery parts. This approach could give us to obtain clear diffraction patterns with high intensity during electrochemical reaction in a short period of time without further relaxation step. We carefully scrutinized reversible structural phase transformations during electrochemical reaction of P2 and O3-layered compounds based on in situ analysis, and detailed results will be discussed.

Structure and stability of BaTiSi2O7

Due to their optical, photo-luminescence (PL), and afterglow properties, barium titanosilicates are compounds of great interest for functional materials and light-emitting devices. Among them, BaTiSi2O7 (BTS2) is certainly one of the most intriguing; it displays peculiar properties (e.g. PL orange emission) whose exhaustive explanation has been hampered to date by the lack of a structure model. In this work, BTS2 and the related compound BaTiSi4O11 (BTS4) were synthesized through conventional solid-state reaction methods. BTS2 invariably shows complex twinning patterns. Thus, its structure solution and Rietveld structure refinement were attempted using synchrotron powder diffraction. BTS2 was found to be an intergrowth of monoclinic and triclinic crystals. The monoclinic phase has the space group P21/n and unit cell a = 7.9836 (3), b = 10.0084 (4), c = 7.4795 (3) Å, and β = 100.321 (3)°, whereas the triclinic phase has the space group and unit cell a = 7.99385 (4), b = 10.01017 (5), c = 7.47514 (3) Å, α = 90.084 (8), β = 100.368 (8) and γ = 89.937 (9)°. These lattices can be seen as a distortion of that of tetragonal synthetic β-BaVSi2O7 with Ti in place of V. The structure models obtained from this study confirm the presence of fivefold coordinated Ti atoms in a distorted pyramidal configuration. The proposed solution supports existing theories for the explanation of the PL orange colour in BTS2.
Supramolecular chemical shift reagents inducing conformational transitions: NMR analysis of carbohydrate homooligomer mixtures

We introduce the concept of supramolecular chemical shift reagents as a tool to improve signal resolution for the NMR analysis of homooligomers. Non-covalent interactions with the shift reagent can constrain otherwise flexible analytes inducing a conformational transition that results in signal separation. Here we use this approach for the quantitative analysis of a complex homooligomeric glycan mixture.

General information
Surface self-assembled hybrid nanocomposites with electroactive nanoparticles and enzymes confined in a polymer matrix for controlled electrocatalysis

A three-dimensional network of highly branched poly(ethyleneimine) (PEI) is designed and synthesized on gold electrode surfaces. A self-assembled monolayer (SAM) of dithiobis(succinimidyl propionate) (DTSP) on a gold electrode was first prepared, which is confirmed by the reductive desorption of Au-S units. The PEI polymer was then covalently immobilized onto the DTSP layer, leaving free primary amine groups acting as a 3D skeleton for high loading of electroactive enzyme-size Prussian blue nanoparticles (PBNPs, 6 nm) via electrostatic trapping. Atomic force microscopy was used to disclose the microscopic structures of the different layers during the surface architecture formation. The resulting surface-bound nanostructured composite shows high electrochemical activity arising from confined PBNPs, and acts as an efficient electrocatalyst towards H$_2$O$_2$ reduction. Facile electron communication is achieved as reflected by a large electron transfer (ET) rate constant ($k_s$) of 200 s$^{-1}$, and the possible electron propagation mechanisms in the polymer network are discussed. This surface/interfacial nanocomposite can be further used in the accommodation of enzymes for electrochemical bio-catalysis. Glucose oxidase (GOD) was used towards this end, in a proof-of-concept study. This enzyme can be co-trapped in the PEI matrix and is interconnected with PBNPs, leading to highly efficient electrocatalytic oxidation and detection of glucose.
Synthesis and characterization of homogeneous interstitial solutions of nitrogen and carbon in iron-based lattices

Since the advent of gaseous nitriding and nitrocarburizing processes in the early 20th-century, numerous process variants and applications have been developed. Improved performance with respect to fatigue, wear and corrosion can be obtained for treated steel components. Despite the advantages and widespread application, the current understanding of the thermodynamics and kinetics governing the processes, as well as the resulting crystal structures and magnetic properties, is still far from complete. An incomplete fundamental description hinders possible process optimization and has motivated the current work in synthesis and characterization of interstitial solutions of nitrogen and carbon in iron-based lattices. In order to avoid the influences of gradients in composition and residual stresses, which are typically found in treated surface layers, homogenous samples are needed. These were prepared from pure iron or austenitic stainless steel using gaseous mixtures of ammonia, hydrogen, acetylene and propene at elevated temperatures. Structural and magnetic properties have been characterized with neutron diffraction, vibrating sample magnetometry and Mössbauer spectroscopy. Thermal decomposition was studied in inert atmospheres with in situ synchrotron X-ray diffraction. Thermal decomposition sequences for iron carbides and carbonitrides, as well as for so-called expanded austenite, were established. In ε-iron nitride, partial substitution of nitrogen by carbon causes an increase in Curie temperature and specific magnetization. Changes in interstitial ordering were deduced from the observed effects on lattice parameters and related to relatively favorable interactions between nitrogen and carbon.

At room temperature expanded austenite is found to be paramagnetic for high and low Nitrogen contents but ferromagnetic for intermediate contents. An anomalous variation in thermal expansion coefficients with interstitial content is caused by spontaneous volume magnetostriction in the ferromagnetic state. Several structural models have previously been proposed for expanded austenite, but all have failed to successfully describe all features of X-ray diffraction data. In the current Evaluation of diffraction data, the effects of stacking faults on hkl-dependent shifts of Bragg reflections were included. Comparison of simulations with experimental data does, however, show that the stacking fault model is not entirely acceptable. The apparent anisotropic deviations from cubic symmetry currently lack an exact quantitative interpretation.

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Synthesis of 1,4,5 trisubstituted γ-lactams via a 3-component cascade reaction

A three component one-pot cascade reaction was developed for the synthesis of 1,4,5-trisubstituted γ-lactams. The resulting scaffold can be modified independently at three positions, two of which are conveniently accessed by changing the components of the one-pot reaction. The phases of building block generation, scaffold synthesis and subsequent appendage modification were adapted to library production, which resulted in a screening library of 500 compounds.

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Synthesis of (Arylamido)pyrrolidinone Libraries through Ritter-Type Cascade Reactions of Dihydroxy lactams

The Ritter-type reaction of arylnitriles and N-acyliminium ions generated in situ from dihydroxy-γ-lactams gave tetrahydropyrrolo[2,3-d]oxazol-5-ones in excellent yields. A subsequent acidic hydrolysis in EtOH/H2O/TFA (trifluoroacetic acid) yielded new (arylamido)pyrrolidinones with excellent cis diastereoselectivity. A combined one-step Ritter–hydrolysis procedure proved to be of equal efficiency. This versatile method, which was successfully used for the construction of a screening library containing 706 molecules within the European Lead Factory consortium, provides a simple way to access new compounds incorporating an arylamido and a pyrrolidinone moiety, both of which are widely found in marketed drugs and in biologically active molecules.

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Molecular libraries of natural product-like and structurally diverse compounds are attractive in early drug discovery campaigns. In here, we present synthetic methodology for library production of hexahydropyrrolo[2,1-a]isoquinoline (HPIQ) compounds. Two advanced HPIQ intermediates, both incorporating two handles for diversification, were synthesized through an oxidative cleavage/Pictet–Spengler reaction sequence in high overall yields. A subsequent metal-catalyzed cross coupling/amidation protocol was developed and its utility in library synthesis was validated by construction of a 20-membered natural product-like molecular library in good overall yields.

General information
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Organisations: Department of Chemistry, Organic Chemistry
Authors: Petersen, R. (Intern), Cohrt, A. E. (Intern), Petersen, M. Á. (Intern), Wu, P. (Intern), Clausen, M. H. (Intern), Nielsen, T. E. (Intern)
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Scopus rating (2016): SJR 0.978 SNIP 0.969 CiteScore 2.96
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Synthesis of Substituted γ- and δ-Lactams through Mannich-Type Reactions of Solid-Supported N-Acyliminium Ions

We report the results of our recent investigations into the reactivity of cyclic solid-supported N-acyliminium ions. An intermolecular Mannich-type transformation of these intermediates was used to generate libraries of substituted lactams. Masked aldehyde building blocks were readily prepared and coupled to peptides immobilized on PEGA800 (polyethylene glycol dimethyl acrylamide) resin through an HMBA [4-(hydroxymethyl)benzoic acid] linker. When treated with acid, the aldehyde was cleanly released and condensed with the amide backbone to form a hydroxylactam/N-acyliminium ion, which underwent intermolecular reactions with a series of nucleophilic heterocycles, such as substituted indoles, thiophenes, furans, and electron-rich benzenes. The resulting lactams were formed within a few minutes and in high purities (typically >85%).
The Dependence of Amyloid-β Dynamics on Protein Force Fields and Water Models

We studied the dynamics of Aβ_{40}, involved in Alzheimer's disease, by using 21 methods combined from Amber03, Amber99sb-ILDN, Charmm27, Charmm22*, OPLS-2001, OPLS-2006, OPLS-2008, Gromos96-43a1, Gromos96-53a6, Gromos96-54a7, and the water models SPC, TIP3P, TIP4P. Major differences in the structural ensembles were systematized: Amber03, Charmm27, and Gromos96-54a7 stabilize the helices; Gromos96-43a1 and Gromos53a6 favor the β-strands (with Charmm22* and Amber99sb-ILDN in between), and OPLS produces unstructured ensembles. The accuracy of the NMR chemical shifts was in the order: Charmm22* > Amber99sb-ILDN > OPLS-2008 > Gromos96-43a1 > Gromos96-54a7 > OPLS-2001 > OPLS-2006 > Gromos96-53a6 > Charmm27 > Amber03. The computed {^3}J_{HN\text{H}α}\-coupling constants were sensitive to experiment type and Karplus parameterization. Overall, the ensembles of Charmm22* and Amber99sb-ILDN provided the best agreement with experimental NMR and circular dichroism data, providing a model for the real Aβ monomer ensemble. Also, the polar water model TIP3P significantly favored helix and compact conformations.
The influence of large-amplitude librational motion on the hydrogen bond energy for alcohol–water complexes

The far-infrared absorption spectra have been recorded for hydrogen-bonded complexes of water with methanol and t-butanol embedded in cryogenic neon matrices at 2.8 K. The partial isotopic substitution of individual subunits enabled by a dual inlet deposition procedure provides for the first time unambiguous assignments of the intermolecular high-frequency out-of-plane and low-frequency in-plane donor OH librational modes for mixed alcohol–water complexes. The vibrational assignments confirm directly that water acts as the hydrogen bond donor in the most stable mixed complexes and the tertiary alcohol is a superior hydrogen bond acceptor. The class of large-amplitude donor OH librational motion is shown to account for up to 5.1 kJ mol⁻¹ of the destabilizing change of vibrational zero-point energy upon intermolecular OH... O hydrogen bond formation. The experimental findings are supported by complementary electronic structure calculations at the CCSD(T)-F12/aug-cc-pVTZ level of theory.

General information

State: Published
Organisations: Department of Chemistry, Lund University
Authors: Andersen, J. (Intern), Heimdal, J. (Ekstern), Larsen, R. W. (Intern)
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Thermodynamic modeling of CO2 absorption in aqueous N-Methyldiethanolamine using Extended UNIQUAC model

A Thermodynamic model that can predict the behavior of the gas sweetening process over the applicable conditions is of vital importance in industry. In this work, Extended UNIQUAC model parameters optimized for the CO2-MDEA-H2O system are presented. Different types of experimental data consisting of pure MDEA vapor pressure, vapor-liquid equilibrium (VLE) (total pressure and CO2 partial pressure), freezing point depression (SLE), excess enthalpy, heat capacity and heat of absorption were used to adjust model parameters. The model was then used to predict the NMR spectroscopic data. The developed model accurately represents thermodynamic and thermal properties of the studied systems. The model parameters are valid in the temperature range from -15 to 200 °C, MDEA mass% of 5-75 and CO2 partial pressure of 0-6161.5 kPa.
Thermodynamic modeling of hydrogen sulfide absorption by aqueous N-methyldiethanolamine using the Extended UNIQUAC model

Aqueous MDEA is the most commonly used solvent for H2S removal from natural gas. A reliable thermodynamic model is required for the proper design of natural gas sweetening processes. In this study, a rigorous thermodynamic model is developed to represent properties of the H2S-MDEA-H2O ternary system. The Extended UNIQUAC model is used to represent the system behavior. The model is created based on models for the constituent binary subsystems. The developed model provides accurate representation of VLE and heat of absorption for the studied system and subsystem in the temperature range of 0-180°C, H2S partial pressure of 0.0033-8329.71kPa, MDEA mass% of 0-50 and loading range of 0-2.17.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, CAPEC-PROCESS, Center for Energy Resources Engineering, Department of Chemistry, CERE – Center for Energy Ressources Engineering
Authors: Sadegh, N. (Intern), Stenby, E. H. (Intern), Thomsen, K. (Intern)
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The SAMENS Method for Gold Nanostructure Syntheses: Green Synthesis and Electrocatalysis

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Organisations: Department of Chemistry, NanoChemistry, Organic Chemistry
Authors: Engelbrekt, C. (Intern), Seselj, N. (Intern), Ulstrup, J. (Intern), Zhang, J. (Intern)
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Relations
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The SAMENS Method for Gold Nanostructure Syntheses: Green Synthesis and Electrocatalysis
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Tin-containing silicates: Alkali salts improve methyl lactate yield from sugars
This study focuses on increasing the selectivity to methyl lactate from sugars using stannosilicates as heterogeneous catalyst. All group I ions are found to have a promoting effect on the resulting methyl lactate yield. Besides, the alkali ions can be added both during the preparation of the catalyst or directly to the solvent mixture to achieve the highest reported yield of methyl lactate (ca. 75%) from sucrose at 170 °C in methanol. The beneficial effect of adding alkali to the reaction media applies not only to highly defect-free Sn-Beta prepared through the fluoride route, but also to materials prepared by post-treatment of dealuminated commercial Beta zeolites, as well as ordered mesoporous stannosilicates, in this case Sn-MCM-41 and Sn-SBA-15. These findings open the door to the possibility of using other preparation methods or different Sn-containing silicates with equally high methyl lactate yields as Sn-Beta.

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Organisations: Department of Chemistry, Organic Chemistry, Haldor Topsoe AS
Authors: Tolborg, S. (Intern), Sádaba, I. (Ekstern), Osmundsen, C. M. (Ekstern), Fristrup, P. (Intern), Holm, M. S. (Ekstern), Taarning, E. (Ekstern)
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Tissue factor activates allosteric networks in factor VIIa through structural and dynamic changes

Background: Tissue factor (TF) promotes colocalization of enzyme (factorVIIa) and substrate (FX or FIX), and stabilizes the active conformation of FVIIa. Details on how TF induces structural and dynamic changes in the catalytic domain of FVIIa to enhance its efficiency remain elusive. Objective: To elucidate the activation of allosteric networks in the catalytic domain of the FVIIa protease it is when bound to TF. Methods: Long-timescale molecular dynamics simulations of FVIIa, free and in complex with TF, were executed and analyzed by dynamic network analysis. Results: Allosteric paths of correlated motion from the TF contact point, Met306, in FVIIa to the active site triad can be described and quantified. In particular, the shortest paths from Met306 to Ser344 and His193 are 16% and 8% longer in free FVIIa than in TF-FVIIa, and they encompass previously undiscovered residue-residue interactions that are not likely to be inferred from mutagenesis studies. Furthermore, paths from Met306 to Ile153 (N-terminus) and Trp364, both representing hallmark residues of allostery, are 7% and 37% longer, respectively, in free FVIIa. Thus, there is significantly weaker coupling between the TF contact point and key residues in the catalytic domain of FVIIa, causing the active site triad to disintegrate in the simulation when TF is not present. Conclusions: These findings complement our current understanding of how the protease FVIIa is stimulated by TF. We demonstrate allosteric networks in the catalytic domain that are activated by TF and help to make FVIIa an efficient catalyst of FIX and FX activation.

General information
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Organisations: Department of Chemistry, Physical and Biophysical Chemistry, Novo Nordisk A/S
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Total synthesis and biochemical evaluation of azumamides A–E and analogs

Histone deacetylases (HDAC) are a family of enzymes, which serve as epigenetic modulators. Their biological function has been related to DNA transcription and regulation of various biochemical pathways. Development of isoform selective HDAC inhibitors could be useful for dissecting the individual biochemical pathways associated with each HDAC isoform and these compounds could potentially serve as anti-cancer drugs. Macrocyclic peptides and depsipeptides is an
interesting class of HDAC inhibitors, which are found in Nature. These compounds are characterized by being highly selective and moderate selective HDAC inhibitors and we turned our attention to a class of cyclic tetrapeptides, known as azumamides. We developed a synthetic route, which allowed us to complete the total synthesis of azumamides A–E. This is the first reported total synthesis of azumamide B–D and our results validate the proposed structures. The key step in this route is a diastereoselective Mannich reaction, which enabled us to prepare two site-specifically edited epimeric azumamide analogs, where the stereochemistry in the unique -amino acid was inverted. The two epimeric homologs were screened together with azumamide A–E against the entire panel of recombinant HDAC isoforms. Thus, providing the first full profiling of the azumamides. The epimers were inactive against the full panel of HDAC enzymes and show that the -amino acid scaffold is highly sensitive to modifications in the stereochemistry. The profiling of the natural products showed that the azumamides are poor inhibitors of class IIa HDACs, but potent inhibitors of HDAC1–3, 10, and 11 (IC50 values between 14 to 67 nM). Furthermore we showed that carboxylic acid containing compounds (azumamide C and E) were more potent than their carboxyamide counterparts (azumamide A and B). Isoform selectivity was observed in class I and class IIb. In class I, azumamides C and E were 60–350-fold more potent towards HDAC1–3 over HDAC8 and in class IIb they were 200-fold more potent against HDAC10 over HDAC6. Finally, we found that azumamide C was 2-fold more potent than azumamide E, which indicate having a tyrosine residue in the macro lactam ring increase the activity compared to the phenylalanine homolog. The synthetic route was elaborated to produce structurally edited azumamide analogs. A series of 2-desmethylated compounds were synthesized in parallel to a series of 2-dimethylated analogs. Having observed the importance of the aromatic amino acid in the azumamides, a tryptophan-series was also prepared. The synthesis of these compounds underline the broad perspective and flexibility of the developed Mannich strategy. The dimethylated analogs were found to be poor HDAC inhibitors and only the tryptophan-containing compound showed activity below 20 μM. The removal of the 2-methyl group induced a 1.5–18-fold loss in potency across the different isoforms. The methyl group was found to be less important for inhibition of HDAC 6 and 8 (1.5–3-fold decrease in activity). Based on NMR solution structures we hypothesize that the 2-methyl group, found in the natural products, guides the 3-side chain towards the active site. Judging from the biochemical data on the dimethylated series, this directing feature is important for the activity of this type of inhibitors. Furthermore, a 3-propyl azumamide C analog was developed in order to investigate the effect of the zinc-binding moiety. Preliminary testing showed that this compound was active against HDAC3 with an IC50 of 3 μM. The straight forward synthesis of the -amino acid required for this analog also illustrate the effectiveness of the developed Mannich reaction. On a different project, a promising Bsmoc-based scaffold was probed to serve as a linker in anti-body drug conjugates (ADC) and preliminary results encourage further investigations of this strategy.
Towards a "Golden Standard" for computing globin stability: Stability and structure sensitivity of myoglobin mutants

Fast and accurate computation of protein stability is increasingly important for e.g. protein engineering and protein misfolding diseases, but no consensus methods exist for important proteins such as globins, and performance may depend on the type of structural input given. This paper reports benchmarking of six protein stability calculators (POPMUSIC 2.1, I-Mutant 2.0, I-Mutant 3.0, CUPSAT, SDM, and mCSM) against 134 experimental stability changes for mutations of sperm-whale myoglobin. Six different high-resolution structures were used to test structure sensitivity that may impair protein calculations. The trend accuracy of the methods decreased as I-Mutant 2.0 (R=0.64-0.65), SDM (R=0.57-0.60), POPMUSIC2.1 (R=0.54-0.57), I-Mutant 3.0 (R=0.53-0.55), mCSM (R=0.35-0.47), and CUPSAT (R=0.25-0.48). The mean signed errors increased as SDM<CUPSAT<I-Mutant 2.0<I-Mutant 3.0<POPMUSIC 2.1<mCSM. Mean absolute errors increased as I-Mutant 2.0<I-Mutant 3.0<POPMUSIC 2.1<CUPSAT<SDM<mCSM. Structural sensitivity increased as I-Mutant 3.0 (0.05)<I-Mutant 2.0 (0.09)<POPMUSIC 2.1 (0.12)<SDM (0.18)<mCSM (0.27)<CUPSAT (0.58). Leaving out heterogeneous experimental data did not change conclusions. The distinct performances reveal room for improvement, but I-Mutant 2.0 is proficient for this purpose, as further validated against a data set of related cytochrome c like proteins. The results also emphasize the importance of high-quality crystal structures and reveal structure-dependent effects even in the near-atomic resolution limit.
Towards a methanol economy based on homogeneous catalysis: methanol to $H_2$ and $CO_2$ to methanol

The possibility to implement both the exhaustive dehydrogenation of aqueous methanol to hydrogen and $CO_2$ and the reverse reaction, the hydrogenation of $CO_2$ to methanol and water, may pave the way to a methanol based economy as part of a promising renewable energy system. Recently, homogeneous catalytic systems have been reported which are able to promote either one or the other of the two reactions under mild conditions. Here, we review and discuss these developments.

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry, University of Rostock
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Web of Science (2016): Indexed yes
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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
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Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
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Web of Science (2012): Indexed yes
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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
Lung infections with *Pseudomonas aeruginosa* (PA) is the most common cause of morbidity and mortality in cystic fibrosis (CF) patients. Due to its ready adaptation to the dehydrated mucosa of CF airways, PA infections tend to become chronic, eventually killing the patient. Hydrogen cyanide (HCN) at ppb level has been reported to be a PA biomarker. For early PA detection in CF children not yet chronically lung infected a non-invasive Surface-Enhanced Raman Spectroscopy (SERS)-based breath nanosensor is being developed. The triple bond between C and N in cyanide, with its characteristic band at $\sim$2133 cm$^{-1}$, is an excellent case for the SERS-based detection due to the infrequent occurrence of triple bonds in nature. For demonstration of direct HCN detection in the gas phase, a gold-coated silicon nanopillar substrate was exposed to 5 ppm HCN in N$_2$. Results showed that HCN adsorbed on the SERS substrate can be consistently detected under different experimental conditions and up to 9 days after exposure. For detection of lower cyanide concentrations serial dilution experiments using potassium cyanide (KCN) demonstrated cyanide quantification down to 1 μM in solution (corresponding to 18 ppb). Lower KCN concentrations of 10 and 100 nM (corresponding to 0.18 and 1.8 ppb) produced SERS intensities that were relatively similar to the reference signal. Since HCN concentration in the breath of PA colonized CF children is reported to be $\sim$13.5 ppb, the detection of cyanide is within the required range.
Transition Metal Catalyzed Reactions for Forming Carbon–Oxygen and Carbon–Carbon Bonds

Dehydrogenative ester formation with a ruthenium NHC complex. A new atom-economical methodology for synthesizing esters by the dehydrogenative coupling of primary alcohols was developed. The reaction is catalyzed by the ruthenium N-heterocyclic carbene complex RuCl2(iiPr)(p-cymene). By screening the effect of different additives, solvents and loadings on the self-condensation of pentanol, the optimal reaction conditions were found to be 2.5 mol % of RuCl2(iiPr)(p-cymene), 4.5 mol % of PCy3 and 10 mol % of KOH in refluxing mesitylene, which gave the ester in nearly quantitative yield by GC analysis. The substrate scope was shown to include a range of different straight-chain and branched primary aliphatic alcohols, which reacted to give the corresponding esters in moderate to excellent yields. Condensation of diols also proceeded well, giving the corresponding lactones in good yields. Benzyl alcohol could be used as substrates, but the yields were generally poor due to decarbonylation of the substrate as a considerable side reaction. Some preliminary mechanistic investigations were performed. The results of these confirmed that the reaction is indeed dehydrogenative with the liberation of two moles of hydrogen per formed mol of ester as assumed. Furthermore a disproportionation mechanism (Tishchenko) could be ruled out due to the fact that free aldehydes did not enter the catalytic cycle. Fast deuterium/hydrogen exchange in the reaction with benzyl alcohol points towards a ruthenium dihydride species being the catalytically active species. A catalytic cycle consistent with these findings, as well as with previous knowledge about this particular catalytic system, was proposed.

2.5 % [Ru] 4.5 % PCy3 10 % KOH mesitylene

O 2 + 2 H2 [Ru] = iii

Synthesis of Anti Zigzag-[5]-phenylene A new member of the family of [5]-phenylenes, named Anti Zigzag-[5]-phenylene, was synthesized and characterized. The desired target molecule was synthesized in ten steps from the commercially available starting material 1,2-dibromobenzene in an overall yield of 0.5 %. Six of the ten steps had not been performed before and six new compounds were isolated and characterized in the process. The target molecule was characterized by HRMS and proton NMR.

Br Br 10 steps 0.5 % Manganese catalyzed radical formation of styryl derivatives A new method for the formation of styryl derivatives by the reaction of ether and hydrocarbon radicals with -bromostyrenes was serendipitously discovered and subsequently optimized. By screening of various radical initiators and transition metal salts the best conditions were found to involve addition of three to four equivalents of Me2Zn to a solution of -bromostyrene, using the radical precursor as solvent, in the presence of 10–12 % of MnCl2, and refluxing overnight in the presence of air. A simple acidic workup and purification by chromatography yielded the products in moderate to good yield. The radical precursor can be a cyclic or acyclic ether or even a cycloalkane, although the latter gives only poor conversion. The -bromostyrene can be substituted with electron-donating or electron-withdrawing substituents in the para position without affecting the yield of the reaction remarkably. The reaction is quenched when TEMPO is added, which confirms that the reaction occurs by a radical mechanism. The reaction is believed to be initiated by the formation of a methyl radical from the reaction of Me2Zn with oxygen. The methyl radical abstracts a hydrogen from the radical precursor and the resulting radical then adds to the -bromostyrene, which subsequently eliminates a bromo radical and forms the product.
Triangular prism-shaped β-peptoid helices as unique biomimetic scaffolds

β-Peptoids are peptidomimetics based on N-alkylated β-aminopropionic acid residues (or N-alkyl-β-alanines). This type of peptide mimic has previously been incorporated in biologically active ligands and has been hypothesized to be able to exhibit foldamer properties. Here we show, for the first time, that β-peptoids can be tuned to fold into stable helical structures. We provide high-resolution X-ray crystal structures of homomeric β-peptoid hexamers, which reveal right-handed helical conformations with exactly three residues per turn and a helical pitch of 9.6-9.8 Å between turns. The presence of folded conformations in solution is supported by circular dichroism spectroscopy showing length- and solvent dependency, and molecular dynamics simulations provide further support for a stabilized helical secondary structure in organic solvent. We thus outline a framework for future design of novel biomimetics that display functional groups with high accuracy in three dimensions, which has potential for development of new functional materials.
Triangular_prism_shaped_b_peptoid_helices_as.pdf
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Source: FindIt
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Triazole-containing N-acyl homoserine lactones targeting the quorum sensing system in Pseudomonas aeruginosa
In an attempt to devise new antimicrobial treatments for biofilm infections, the bacterial cell-cell communication system termed quorum sensing has emerged as an attractive target. It has proven possible to intercept the communication system by synthetic non-native ligands and thereby lower the pathogenesis and antibiotic tolerance of a bacterial biofilm. To identify the structural elements important for antagonistic or agonistic activity against the Pseudomonas aeruginosa LasR protein, we report the synthesis and screening of new triazole-containing mimics of natural N-acyl homoserine lactones. A series of azide- and alkyne-containing homoserine lactone building blocks was used to prepare an expanded set of 123 homoserine lactone analogues through a combination of solution- and solid-phase synthesis methods. The resulting compounds were subjected to cell-based quorum sensing screening assays, thereby revealing several bioactive compounds, including 13 compounds with antagonistic activity and 9 compounds with agonistic activity. (C) 2015 Elsevier Ltd. All rights reserved.

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Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.01 SNIP 1.101 CiteScore 2.87
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.063 SNIP 1.21 CiteScore 3.08
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.2 SNIP 1.312 CiteScore 3.12
This paper reports the identification, heterologous expression in *Escherichia coli* and characterization of TtMCO from the thermophilic bacterium *Thermobaculum terrenum*, the first laccase-like multi-copper oxidase (LMCO) from the distinct Phylum Chloroflexi. TtMCO has only 39% identity to its closest characterized homologue, CotA from *Bacillus subtilis*, but sequence and spectrophotometry confirmed copper coordination similar to that of LMCOs. TtMCO is extremely thermophilic with a half-time of inactivation of 2.24 days at 70°C and 350 min at 80°C and pH 7, consistent with a hyperthermal habitat of the host. TtMCO was screened for activity against 56 chemically diverse substrates. It displayed limited activity on classical LMCO substrates, such as e.g. phenolics, transition metals, or bilirubin. Highest activities were observed for nitrogen-containing aromatic compounds, i.e. 1.8-diaminonaphtalene (K_m = 0.159 mM, k_cat = 0.295 s\(^{-1}\)) and ABTS (K_m = 0.844mM, k_cat = 2.13 s\(^{-1}\)). The combined data suggest a distinct role of TtMCO and a substantial trade-off between activity and stability, compared to other characterized bacterial LMCOs, making it of interest in future protein engineering studies.
Tuning the composition of metastable Co$_x$Ni$_y$Mg$_{100-x-y}$O(OH)(OCH$_3$) nanoplates for optimizing robust methane dry reforming catalyst

Finding controllable, low-cost, and scalable ways to generate Ni-based catalysts is the bottleneck for methane dry reforming catalyst design. A new method for generating trimetallic Co$_x$Ni$_y$Mg$_{100-x-y}$O solid solution platelets enclosed by (111) facets has been developed from the topotactic pyrolysis of the metastable precursor Co$_x$Ni$_y$Mg$_{100-x-y}$O(OH)(OCH$_3$) derived from solvothermal synthesis. The catalyst composition and reaction conditions have been modulated to achieve maximum coke resistance and catalyst stability. Long-term stability for 1000 h time on stream at 800°C has been achieved for the optimized Co$_{0.075}$Ni$_{7.425}$Mg$_{92.5}$O catalyst. The role of Co in the catalyst has been disclosed through kinetic measurements and detailed characterization of the spent catalysts. Co is enriched on the Co-Ni alloy surface under reforming conditions and accelerates the gasification of coke intermediates. Co also enhances the chemisorption of oxygen and reduces the activation energy for methane fragmentation, which is the rate-determining step for the overall reaction.

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Scopus rating (2012): SJR 3.005 SNIP 2.277 CiteScore 6.17
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BFI (2010): BFI-level 2
Scopus rating (2010): SJR 3.376 SNIP 2.213
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.951 SNIP 2.158
Visualizing the non-equilibrium dynamics of photoinduced intramolecular electron transfer with femtosecond X-ray pulses

Ultrafast photoinduced electron transfer preceding energy equilibration still poses many experimental and conceptual challenges to the optimization of photoconversion since an atomic-scale description has so far been beyond reach. Here we combine femtosecond transient optical absorption spectroscopy with ultrafast X-ray emission spectroscopy and diffuse X-ray scattering at the SACLA facility to track the non-equilibrated electronic and structural dynamics within a bimetallic donor–acceptor complex that contains an optically dark centre. Exploiting the 100-fold increase in temporal resolution as compared with storage ring facilities, these measurements constitute the first X-ray-based visualization of a non-equilibrated intramolecular electron transfer process over large interatomic distances. Experimental and theoretical results establish that mediation through electronically excited molecular states is a key mechanistic feature. The present study demonstrates the extensive potential of femtosecond X-ray techniques as diagnostics of non-adiabatic electron transfer processes in synthetic and biological systems, and some directions for future studies, are outlined.

General information
State: Published
Organisations: Department of Physics, Neutrons and X-rays for Materials Physics, Center for Atomic-scale Materials Design, Department of Chemistry, Physical and Biophysical Chemistry, Lund University, University of Copenhagen, Hungarian Academy of Sciences, High Energy Accelerator Research Organization, The Hamburg Centre for Ultrafast Imaging, European XFEL, Argonne National Laboratory, The Institute of Chemical and Physical Research, Japan Synchrotron Radiation Research Institute
Number of pages: 10
Publication date: 2015
Main Research Area: Technical/natural sciences

Publication information
Xylose Isomerization with Zeolites in a Two-Step Alcohol–Water Process

Isomerization of xylose to xylulose was efficiently catalyzed by large-pore zeolites in a two-step methanol–water process that enhanced the product yield significantly. The reaction pathway involves xylose isomerization to xylulose, which, in part, subsequently reacts with methanol to form methyl xyluloside (step 1) followed by hydrolysis after water addition to form additional xylulose (step 2). NMR spectroscopy studies performed with 13C-labeled xylose confirmed the proposed reaction pathway. The most active catalyst examined was zeolite Y, which proved more active than zeolite beta, ZSM-5, and mordenite. The yield of xylulose obtained over H-USY (Si/Al=6) after 1 h of reaction at 100°C was 39%. After water hydrolysis in the second reaction step, the yield increased to 47%. Results obtained from pyridine adsorption studies confirm that H-USY (6) is a catalyst that combines Brønsted and Lewis acid sites, and isomerizes xylose in alcohol media to form xylulose at low temperature. The applied zeolites are commercially available; do not contain any auxiliary tetravalent metals, for example, tin, titanium, or zirconium; isomerize xylose efficiently; are easy to regenerate; and are prone to recycling.

General information

State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Universidad Rey Juan Carlos
Authors: Paniagua, M. (Ekstern), Shunmugavel, S. (Intern), Melián Rodriguez, M. (Intern), Melero, J. A. (Ekstern), Riisager, A. (Intern)
Number of pages: 7
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Journal: ChemSusChem (Print)
Volume: 8
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BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
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
Scopus rating (2011): SJR 2.767 SNIP 1.504 CiteScore 5.53
ISI indexed (2011): ISI indexed no
Web of Science (2011): Indexed yes
Scopus rating (2010): SJR 1.945 SNIP 1.134
Web of Science (2010): Indexed yes
Scopus rating (2009): SJR 0.973 SNIP 0.72
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.291 SNIP 0.48
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.273 SNIP 0.495
Scopus rating (2006): SJR 0.243 SNIP 0.372
Scopus rating (2005): SJR 0.195 SNIP 0.285
Scopus rating (2004): SJR 0.214 SNIP 0.276
Scopus rating (2003): SJR 0.276 SNIP 0.419
Scopus rating (2002): SJR 0.312 SNIP 0.586
Scopus rating (2001): SJR 0.292 SNIP 0.496
Scopus rating (2000): SJR 0.422 SNIP 0.556
Scopus rating (1999): SJR 0.511 SNIP 0.708
Original language: English
Alcohols, Heterogeneous catalysis, Isomerization, NMR spectroscopy, Zeolites
DOIs:
10.1002/cssc.201402965
Source: PublicationPreSubmission
Source-ID: 105957389
Publication: Research - peer-review › Journal article – Annual report year: 2015
Absorption of Flue-Gas Components by Ionic Liquids

Gas separation by ionic liquids (ILs) is a promising new research field with several potential applications of industrial interest. Thus cleaning of industrial off gases seems to be attractive by use of ILs and Supported Ionic Liquid Phase (SILP) materials. The potential of selected ILs for absorption of NOX, CO2 and SO2 are demonstrated and the possible mechanism of absorption described on the molecular level. Special focus regards the interaction of the ILs with water vapor, which is an important feature in envisaged application of flue gas cleaning in power plants, waste incineration plants, cement and glass factories as well as on board ships.

General information

State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Université Paul Cezanne
Authors: Kolding, H. (Intern), Thomassen, P. L. (Intern), Mossin, S. (Intern), Kegnæs, S. (Intern), Riisager, A. (Intern), Rogez, J. (Ekstern), Mikaelian, G. (Ekstern)
Pages: 97-108
Publication date: 2014
Conference: 226th Meeting of the Electrochemical Society (ECS) and 7th Meeting of the Mexico Section of the Electrochemical Society ECS and SMEQ Joint International Meeting, Cancun, Mexico, 05/10/2014 - 05/10/2014
Main Research Area: Technical/natural sciences

Publication information

Journal: ECS Transactions
Volume: 64
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Ratings:
BFI (2018): BFI-level 1
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
Scopus rating (2009): SJR 0.241 SNIP 0.266
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.253 SNIP 0.25
Scopus rating (2007): SJR 0.213 SNIP 0.206
Scopus rating (2006): SJR 0.135 SNIP 0.062
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Source: PublicationPreSubmission
Source-ID: 105210803
Publication: Research - peer-review › Conference article – Annual report year: 2015
Acetalization of furfural with zeolites under benign reaction conditions

Acetalization is a viable method to protect carbonyl functionalities in organic compounds and offers a potential synthetic strategy for synthesizing derived chemicals. In this work, several families of commercial zeolites have been employed as solid acid catalysts in the acetalization of furfural to form furfural diethyl acetal at room temperature using ethanol as a renewable solvent. Among the tested catalysts, H-USY (6) provided the highest catalytic activity (79% acetal yield), excellent selectivity and reusability in five consecutive reaction runs. Process parameters such as, e.g. reaction time, catalyst loading and applicability of different lower alcohols were evaluated and optimized.

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Universidad de Malaga
Authors: Rubio-Caballeroa, J. M. (Ekstern), Shunmugavel, S. (Intern), Maireles-Torres, P. (Ekstern), Riisager, A. (Intern)
Pages: 233-236
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Journal: Catalysis Today
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Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.26 SJR 1.312 SNIP 1.363
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.316 SNIP 1.413 CiteScore 4
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.316 SNIP 1.474 CiteScore 3.72
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.307 SNIP 1.432 CiteScore 3.39
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.475 SNIP 1.437 CiteScore 3.38
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.479 SNIP 1.526 CiteScore 3.34
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.763 SNIP 1.465
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.716 SNIP 1.644
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.684 SNIP 1.543
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.589 SNIP 1.598
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.51 SNIP 1.326
Adsorption Dynamics and Self-Assembled L-cysteine on Au(100)

As the only amino acid with a functional thiol group, L-cysteine offers a strong perspective both for binding to gold and other metals, and for gentle immobilization of biomolecules. Binding to single-crystal, atomically planar surfaces offers the additional perspective that bound L-cysteine can be structurally mapped at the single-molecule level. In this work, we have followed the adsorption of L-cysteine on single-crystal Au(100) by measuring the electrode potential dynamics during the adsorption process. In situ STM revealed the structure of the self-assembled ordered layers. The molecular assemblies were studied through simulated STM image contrast based on density functional theory (DFT) including solvation effects. The adsorption kinetics showed clearly a complex pattern with at least one intermediate state. The modelling disclosed details of the interaction of all functional groups with the Au(100)-substrate.

Alternative catalysts and technologies for NOx removal from biomass- and wastefired plants.

The objective of this thesis has been to investigate alternative catalysts and technologies which are able to handle the challenging gases from biomass- and waste-red units. Nitrogen oxides are unwanted by-products formed to some extent during almost any combustion. These by-products are usually removed with the selective catalytic reduction (SCR) using a vanadia-tungsta-titania (VWT) catalyst and ammonia (NH3) as reductant. For application in coal- and gas-red power plants this technology is mature. However, when ring biomass the flue gas contains potassium in large amounts which deactivates the VWT catalyst very rapidly. Firing of biomass increased strongly over the past decade and is expected to increase even further in the near future. Also waste incineration creates flue gases that are very challenging to the SCR catalyst. Therefore, SCR units in waste incineration plants are commonly placed at the so-called tail-end position, just before being released through the stack. At this position, the flue gas is very clean, so the catalyst has a long lifetime. However, tail-end placement usually requires costly reheating of the flue gas. Two approaches were undertaken to solve the alkali poisoning problem: Use of Ag/Al2O3 as catalyst with hydrocarbons (ethanol, propene) as reductants (HCSCR), and by developing low-temperature catalysts for NH3-SCR to be used in the tail-end position at 150 C, making costly reheating redundant. The hope that HC-SCR is insensitive to potassium has been in vain. The deNOx activity over Ag/Al2O3 used in ethanol-SCR is practically as much reduced as in the NH3-SCR case over the traditional VWT catalyst. Furthermore, poisoning with potassium leads to unselective oxidation of the hydrocarbons instead of NO reduction and SO2 concentrations as low as 20 ppm can heavily deactivate the Ag/Al2O3 catalyst. Therefore we concluded that HC-SCR is unt for potassium containing flue gases. The efforts at developing a catalyst to be used at the tail end position were more fruitful and culminated in a patent application due to which only limited information can be disclosed. At 150 C, in the
presence of 10 % H2O, the catalyst under patenting matches the activity of the commercial VWT one at 220 C. However, 
uo gases at the tail-end position can contain up to 20 % H2O, increasing the temperature of activity parity to 180 C. 
Furthermore, the catalyst is also sensitive to SO2, even at low concentrations. One of the causes for the catalyst's high 
activity in NO reduction, the high concentration of chemisorbed surface oxygen, might be exploited in the removal of 
volatile organic compounds (VOC), another growing environmental technology. Preliminary tests are under planning.

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Department of Chemical and 
Biochemical Engineering, CHEC Research Centre
Authors: Schill, L. (Intern), Fehrmann, R. (Intern), Jensen, A. D. (Intern)
Number of pages: 195
Publication date: 2014

Amine-Functionalized Amino Acid-based Ionic Liquids as Efficient and High-Capacity Absorbents for CO2

Ionic liquids (ILs) comprised of ammonium cations and anions of naturally occurring amino acids containing an additional 
amine group (e.g., lysine, histidine, asparagine, and glutamine) were examined as high-capacity absorbents for CO2. An 
absorption capacity of 2.1 mol CO2 per mol of IL (3.5 mol CO2 per kg IL, 13.1 wt% CO2) was measured for [N66614][Lys] 
at ambient temperature and about 1 mol CO2 per mol of IL at 808C (under 1 bar of CO2). This demonstrated that 
desorption is possible under CO2-rich conditions by temperature-swing absorption; three consecutive sorption cycles were 
performed with the IL. The mechanistic and kinetic study of the absorption process was further substantiated by NMR 
spectroscopy and in situ attenuated total reflectance FTIR for [N66614][Lys] and the homologous phosphonium-based IL 
[P66614][Lys]. This study revealed that carbamic acid was formed with CO2 in both ILs by chemisorption; 
however, the amino acid–carboxyl groups on the anion played an important—but different—catalytic role for 
the sorption kinetics in the two ILs. The origin of the cationic effect is speculated to be correlated with the strength of the 
ion interactions in the two ILs.

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Authors: Shunmugavel, S. (Intern), Kunov-Kruse, A. J. (Intern), Fehrmann, R. (Intern), Riisager, A. (Intern)
Pages: 897-902
Publication date: 2014
Main Research Area: Technical/natural sciences

Publication information
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Volume: 7
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ISSN (Print): 1864-5631
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BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
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
A Model of Proteostatic Energy Cost and Its Use in Analysis of Proteome Trends and Sequence Evolution.

A model of proteome-associated chemical energetic costs of cells is derived from protein-turnover kinetics and protein folding. Minimization of the proteostatic maintenance cost can explain a range of trends of proteomes and combines both protein function, stability, size, proteostatic cost, temperature, resource availability, and turnover rates in one simple framework. We then explore the ansatz that the chemical energy remaining after proteostatic maintenance is available for reproduction (or cell division) and thus, proportional to organism fitness. Selection for lower proteostatic costs is then shown to be significant vs. typical effective population sizes of yeast. The model explains and quantifies evolutionary conservation of highly abundant proteins as arising both from functional mutations and from changes in other properties such as stability, cost, or turnover rates. We show that typical hypomorph mutations can be selected against due to increased cost of compensatory protein expression (both in the mutated gene and in related genes, i.e. epistasis) rather than compromised function itself, although this compensation depends on the protein's importance. Such mutations exhibit larger selective disadvantage in abundant, large, synthetically costly, and/or short-lived proteins. Selection against increased turnover costs of less stable proteins rather than misfolding toxicity per se can explain equilibrium protein stability distributions, in agreement with recent findings in E. coli. The proteostatic selection pressure is stronger at low metabolic rates (i.e. scarce environments) and in hot habitats, explaining proteome adaptations towards rough environments as a question of energy. The model may also explain several trade-offs observed in protein evolution and suggests how protein properties can coevolve to maintain low proteostatic cost.
A mutant sialidase having trans-sialidase activity for use in production of sialylated glycans

The invention provides a mutant enzyme having trans-sialidase activity (EC 3.2.1.18), characterized by an enhanced trans-sialidase:sialidase ratio when compared to its parent sialidase enzyme. Further the enzyme may be used in a method for trans-sialylating mono- and oligo-saccharides, including galacto-oligosaccharides (GOS), fructo-oligosaccharides (FOS), malto-oligosaccharides (MOS), isomalto-oligosaccharides (IMO), lactulose, melibiose, maltose, glycosyl sucrose, lactosucrose and fucose. Trans-sialylated mono- and oligo-saccharides, produced with the mutant enzyme, are useful in preparing infant formula, a prebiotic nutritional supplement, and a food supplement.

General information
An add-on cap for ATR-IR spectroscopy studies
The invention relates to a cap (300B) for an attenuated total reflectance infrared (ATR-IR) spectrometer, the ATR-IR spectrometer comprising an ATR-IR plate (200). The cap (300B) comprises an ATR-IR plate facing cap surface. When the ATR-IR plate facing cap surface is placed on the sample surface side of the ATR-IR plate (200), a sample cavity enclosing the sample is formed between the sample surface side of the ATR-IR plate (200) and the ATR-IR plate facing cap surface of the cap (300B). This sample cavity can be an air tight cavity. The cap may further comprise a bridge (322), which functions as cap securing means (322), as the cap (300B) is secured onto the ATR-IR plate (200) by a pressure clamp (108) and an arm (110) holding the pressure clamp (108) pressing on the bridge (322).

General information
State: Published
Organisations: Department of Chemistry
Authors: Kunov-Kruse, A. J. (Intern), Thomsen, J. (Intern), Piltoft, J. S. (Intern), Petersen, C. N. (Intern)
Publication date: 2014

An add-on system for photochemical ATR-IR spectroscopy studies
The invention relates to an add-on system for a unit mainly adapted for attenuated total reflectance infrared (ATR-IR) spectroscopy. The add-on system enables time-resolved in-situ measurements of different sample types in an easy, simple and inexpensive way. The add-on system includes a cap (300G,300H,300J) to be attached to an ATR plate (200) to form a sample cavity (302) enclosing the sample (204). The cap (300G,300H,300J) comprises openings for allowing gas to enter and exit the sample cavity (304,306,308), cap sealing means (310) for providing a tight sealing between the ATR plate (200) and the cap (300B,300H,300J), a source of light, e.g. a light emitting diode (418) or an optical fibre (416) connectable to a laser, and a light source containing cavity.

General information
State: Published
Organisations: Department of Chemistry
Authors: Kunov-Kruse, A. J. (Intern), Thomsen, J. (Intern), Piltoft, J. S. (Intern), Petersen, C. N. (Intern)
Publication date: 2014
An add-on system including a micro-reactor for an atr-ir spectrometer
The invention relates to an add-on system for an attenuated total reflectance infrared (ATR-IR) spectrometer, the add-on system allowing for time-resolved in situ IR measurements of heterogeneous mixtures. The add-on device comprises a micro-reactor (300A) forming a sample cavity (305) when the micro-reactor (300A) is placed on a sample surface side of an ATR-IR plate (200), a sample magnet (312) being adapted for being placed in the sample cavity (305), and a magnet system (400) comprising an outer magnet (402), the magnet system (400) being adapted for rotating the outer magnet (402) in a plane being substantially parallel to the plane in which the ATR-IR plate (200) lies, wherein, when the micro-reactor (300A) is placed on the ATR-IR plate (200), the outer magnet (402) is adapted for rotating the sample magnet (312) inside the sample cavity (305).

Analysis of an industrial production suspension of Bacillus lentus subtilisin crystals by powder diffraction: a powerful quality-control tool
A microcrystalline suspension of Bacillus lentus subtilisin (Savinase) produced during industrial large-scale production was analysed by X-ray powder diffraction (XRPD) and X-ray single-crystal diffraction (MX). XRPD established that the bulk microcrystal sample representative of the entire production suspension corresponded to space group P212121, with unit-cell parameters a = 47.65, b = 62.43, c = 75.74 Å, equivalent to those for a known orthorhombic crystal form (PDB entry 1ndq). MX using synchrotron beamlines at the Diamond Light Source with beam dimensions of 20 × 20 µm was subsequently used to study the largest crystals present in the suspension, with diffraction data being collected from two single crystals (~20 × 20 × 60 µm) to resolutions of 1.40 and 1.57 Å, respectively. Both structures also belonged to space group P212121, but were quite distinct from the dominant form identified by XRPD, with unit-cell parameters a = 53.04, b = 57.55, c = 71.37 Å and a = 52.72, b = 57.13, c = 65.86 Å, respectively, and refined to R = 10.8% and Rfree = 15.5% and to R = 14.1% and Rfree = 18.0%, respectively. They are also different from any of the forms previously reported in the PDB. A controlled crystallization experiment with a highly purified Savinase sample allowed the growth of single crystals of the form identified by XRPD; their structure was solved and refined to a resolution of 1.17 Å with an R of 9.2% and an Rfree of 11.8%. Thus, there are at least three polymorphs present in the production suspension, albeit with the 1ndq-like microcrystals predominating. It is shown how the two techniques can provide invaluable and complementary information for such a production suspension and it is proposed that XRPD provides an excellent quality-control tool for such suspensions.

General information
State: Published
Organisations: Department of Chemistry, X-ray Crystallography, University of York, Novozymes A/S
Authors: Frankær, C. G. (Intern), Moroz, O. V. (Ekstern), Turkenburg, J. P. (Ekstern), Aspmo, S. I. (Ekstern), Thymark, M. (Ekstern), Friis, E. P. (Ekstern), Ståhl, K. (Intern), Nielsen, J. E. (Ekstern), Wilson, K. S. (Ekstern), Harris, P. (Intern)
Pages: 1115–1123
Publication date: 2014
Main Research Area: Technical/natural sciences
Publication information
Journal: Acta Crystallographica. Section D: Biological Crystallography
Volume: 70
Issue number: Part 4
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Analytical, 1-Dimensional Impedance Model of a Composite Solid Oxide Fuel Cell Cathode

An analytical, 1-dimensional impedance model for a composite solid oxide fuel cell cathode is derived. It includes geometrical parameters of the cathode, e.g., the internal surface area and the electrode thickness, and also material parameters, e.g., the surface reaction rate and the vacancy diffusion coefficient. The model is successfully applied to a total of 42 impedance spectra, obtained in the temperature range 555°C–852°C and in the oxygen partial pressure range 0.028 atm–1.00 atm for a cathode consisting of a 50/50 wt% mixture of (La0.6Sr0.4)0.99CoO3 − δ and Ce0.9Gd0.1O1.95 − δ. The surface exchange coefficient in oxygen for T = 802°C and [Formula] is found to be kEx = 1.42 × 10− 4 m s− 1 and with an activation energy of Ea = 107 kJ mol− 1, in fair agreement with literature. A parameter variation and a steady state analysis is performed, verifying the soundness of the model and providing both qualitative and quantitative information on the evolution of the impedance spectra of cathodes with changing parameters.
An azumamide C analogue without the zinc-binding functionality

Histone deacetylase (HDAC) inhibitors have attracted considerable attention due to their promise as therapeutic agents. Most HDAC inhibitors adhere to a general "cap-linker-Zn2+-binding group" architecture but recent studies have indicated that potent inhibition may be achieved without a Zn2+-coordinating moiety. Herein, we describe the synthesis of an azumamide analogue lacking its native Zn2+-binding group and evaluation of its inhibitory activity against recombinant human HDAC1–11. Furthermore, kinetic investigation of the inhibitory mechanism of both parent natural product and synthetic analogue against HDAC3-NCoR2 is reported as well as their activity against Burkitt's lymphoma cell proliferation.

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry, University of Copenhagen, Statens Serum Institut
Authors: Villadsen, J. (Intern), Kitir, B. (Intern), Wich, K. (Ekstern), Friis, T. (Ekstern), Madsen, A. S. (Intern), Olsen, C. A. (Intern)
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Main Research Area: Technical/natural sciences

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BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.896 SNIP 0.728 CiteScore 2.49
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.946 SNIP 0.736 CiteScore 2.38
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.941 SNIP 0.779 CiteScore 2.41
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.978 SNIP 0.741 CiteScore 2.57
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.031 SNIP 0.942 CiteScore 2.56
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
A new approach to model strain change of gelled waxy crude oil under constant stress

Deformation of gelled waxy crude oil with loaded stress is worthy of research for the flow assurance of pipelining system. A dispersion parameter was introduced to characterize the disruption degree of wax crystal structure in crude oil with shear action. Based on fractional calculus theory, a rheological model incorporating dispersion parameter was proposed to describe creep of gelled waxy crude. A discrete and numerical algorithm was proposed to solve the model. Combining with the experimental results of five kinds of waxy crude oil, the model parameters were regressed and found to change monotonously with test temperature. Multiple creep curves of gelled waxy crude oil at a certain temperature can be described with this model.
A new insight into the zinc-dependent DNA-cleavage by the colicin E7 nuclease: a crystallographic and computational study.

The nuclease domain of colicin E7 metallonuclease (NCoIE7) contains its active centre at the C-terminus. The mutant ΔN4-NCoIE7-C* - where the four N-terminal residues including the positively charged K446, R447 and K449 are replaced with eight residues from the GST tag - is catalytically inactive. The crystal structure of this mutant demonstrates that its overall fold is very similar to that of the native NCoIE7 structure. This implicates the stabilizing effect of the remaining N-terminal sequence on the structure of the C-terminal catalytic site and the essential role of the deleted residues in the mechanism of the catalyzed reaction. Complementary QM/MM calculations on the protein-DNA complexes support the less favourable cleavage by the mutant protein than by NCoIE7. Furthermore, a water molecule as a possible ligand for the Zn(2+)-ion is proposed to play a role in the catalytic process. These results suggest that the mechanism of the Zn(2+)-containing HNH nucleases needs to be further studied and discussed.

General information
State: Published
Organisations: Department of Chemistry, Metalloprotein Chemistry and Engineering, MTA-SZTE Bioinorganic Chemistry Research Group, University of Szeged, University of Copenhagen, Academy of Sciences of the Czech Republic, University of Tsukuba
Authors: Czene, A. (Ekstern), Tóth, E. (Ekstern), Németh, E. (Ekstern), Otten, H. (Ekstern), Poulsen, J. N. (Ekstern), Christensen, H. E. M. (Intern), Rulíšek, L. (Ekstern), Nagata, K. (Ekstern), Larsen, S. (Ekstern), Gyurcsik, B. (Ekstern)
Pages: 2090-2099
Publication date: 2014
Main Research Area: Technical/natural sciences

Publication information
Journal: Metallomics
Volume: 6
Issue number: 11
ISSN (Print): 1756-5901
Ratings:
BFI (2018): BFI-level 1
An improved method of preparation of nanoparticular metal oxide catalysts

The present invention concerns an improved method of preparation of nanoparticular vanadium oxide/anatase titania catalysts having a narrow particle size distribution. In particular, the invention concerns preparation of nanoparticular vanadium oxide/anatase titania catalyst precursors comprising combustible crystallization seeds upon which the catalyst metal oxide is coprecipitated with the carrier metal oxide, which crystallization seeds are removed by combustion in a final calcining step.

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Authors: Kristensen, S. B. (Intern), Kunov-Kruse, A. J. (Intern), Riisager, A. (Intern), Fehrmann, R. (Intern)
Publication date: 2014

Publication information
IPC: B01J21/06
Patent number: WO2014170222
Date: 23/10/2014
Priority date: 17/04/2013
Priority number: EP20130164087
Original language: English
Main Research Area: Technical/natural sciences
Publication: Research › Patent – Annual report year: 2014

An Improved Protocol for the Synthesis of 1-(Mesitylenesulfonyl)-3-nitro-1,2,4-triazole (MSNT)

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry
Authors: Petersen, R. (Intern), Jensen, J. F. (Intern), Nielsen, T. E. (Intern)
Pages: 267-271
Publication date: 2014
A Photolabile Linker for the Solid-Phase Synthesis of Peptide Hydrazides and Heterocycles

A photolabile hydrazine linker for the solid-phase synthesis of peptide hydrazides and hydrazine-derived heterocycles is presented. The developed protocols enable the efficient synthesis of structurally diverse peptide hydrazides derived from the standard amino acids, including those with side-chain protected residues at the C-terminal of the resulting peptide hydrazide, and are useful for the synthesis of dihydropyrano[2,3-c]pyrazoles. The linker is compatible with most commonly used coupling reagents and protecting groups for solid-phase peptide synthesis.
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)
Pages: 8645-8648
Publication date: 2014
Main Research Area: Technical/natural sciences

Publication information
Journal: ANGEWANDTE CHEMIE-INTERNATIONAL EDITION
Volume: 53
Issue number: 33
ISSN (Print): 1433-7851
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
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
A short designed semi-aromatic organic nanotube – synthesis, chiroptical characterization, and host properties

The first generation of an organic nanotube based on the enantiomerically pure bicyclo[3.3.1]nonane framework is presented. The helical tube synthesised is the longest to date having its aromatic systems oriented parallel to the axis of propagation (length 26 Å and inner diameter 11 Å according to molecular dynamics simulations in chloroform). The synthesis of the tube, a heptamer, is based on a series of Friedländer condensations and the use of pyrido[3,2-d]pyrimidine units as masked 2-amino aldehydes, as a general means to propagate organic tubular structures and the introduction of a methoxy group for modification toward solubility and functionalization are described. The electronic CD spectra of the tube and molecular intermediates are correlated with theoretical spectra calculated with time-dependent density functional theory to characterize the chirality of the tube. Both experimental (NMR-titrations) and theoretical (molecular dynamics simulations) techniques are used to investigate the use of the tube as a receptor for the acetylcholine and guanidinium cations, respectively.

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry, Lund University
Authors: Wixe, T. (Ekstern), Christensen, N. J. (Intern), Lidin, S. (Ekstern), Fristrup, P. (Intern), Wärnmark, K. (Ekstern)
Pages: 8930-8941
Publication date: 2014
Main Research Area: Technical/natural sciences

Publication information
Journal: Organic & Biomolecular Chemistry
Volume: 12
A study on the electrochemical behaviour of polypyrrole films in concentrated aqueous alkali halide electrolytes

The electrochemical behaviour of polypyrrole films doped with dodecyl benzene sulfonate (PPy/DBS) in LiCl aqueous electrolytes has been investigated in order to find the electrolyte concentration suitable for the operation of PPy/DBS-
based soft actuators. For this investigation, PPy/DBS films deposited on gold-coated quartz crystals by electropolymerization and simultaneous cyclic voltammetry and electrochemical quartz crystal microbalance techniques were used. During the first redox cycle, while large water movement is observed along with the counter ions in dilute electrolytes, such water transport in concentrated electrolytes is found to be very low. In dilute electrolytes, water molecules accompany counter ions as solvated molecules and due to osmotic effect. In concentrated electrolytes, water movement is less due to limited availability of free water as well as a smaller osmotic pressure difference. In highly concentrated aqueous electrolytes, the mass of the PPy/DBS film at the end of each redox cycle is found to drift, which can be controlled by changing the concentration of the electrolyte. The PPy/DBS films were also cycled at different scan rates in various alkali halide aqueous electrolytes of concentrations 0.1 and 1 M to determine the effective diffusion coefficients of alkali ions in the films. The effective diffusion coefficients were found to increase with the concentration of the electrolytes and decrease with the increase in size of cations.

General information
State: Published
Organisations: Department of Chemistry, Physical and Biophysical Chemistry, South Eastern University of Sri Lanka, University of Malaya
Authors: Jafeen, M. J. M. (Ekstern), Careem, M. (Ekstern), Skaarup, S. (Intern)
Pages: 535-544
Publication date: 2014
Main Research Area: Technical/natural sciences

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Journal: Ionics
Volume: 20
Issue number: 4
ISSN (Print): 0947-7047
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.92 SJR 0.504 SNIP 0.634
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.479 SNIP 0.645 CiteScore 1.85
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.44 SNIP 0.692 CiteScore 1.7
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.471 SNIP 0.937 CiteScore 1.71
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.59 SNIP 1.023 CiteScore 1.62
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.525 SNIP 0.76 CiteScore 1.34
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.497 SNIP 0.604
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.547 SNIP 0.612
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.326 SNIP 0.424
Scopus rating (2007): SJR 0.25 SNIP 0.363
Scopus rating (2006): SJR 0.214 SNIP 0.24
Bacteria-Triggered Release of Antimicrobial Agents

Medical devices employed in healthcare practice are often susceptible to microbial contamination. Pathogenic bacteria may attach themselves to device surfaces of catheters or implants by formation of chemically complex biofilms, which may be the direct cause of device failure. Extracellular bacterial lipases are particularly abundant at sites of infection. Herein it is shown how active or proactive compounds attached to polymeric surfaces using lipase-sensitive linkages, such as fatty acid esters or anhydrides, may be released in response to infection. Proof-of-concept of the responsive material is demonstrated by the bacteria-triggered release of antibiotics to control bacterial populations and signaling molecules to modulate quorum sensing. The self-regulating system provides the basis for the development of device-relevant polymeric materials, which only release antibiotics in dependency of the titer of bacteria surrounding the medical device.

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry, University of Copenhagen
Authors: Komnatnyy, V. V. (Intern), Chiang, W. (Ekstern), Tolker-Nielsen, T. (Ekstern), Givskov, M. C. (Ekstern), Nielsen, T. E. (Intern)
Pages: 449-451
Publication date: 2014
Main Research Area: Technical/natural sciences

Publication information
Journal: Angewandte Chemie
Volume: 126
Issue number: 2
ISSN (Print): 0044-8249
Ratings:
BFI (2018): BFI-level 1
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
Bacteria-Triggered Release of Antimicrobial Agents

Medical devices employed in healthcare practice are often susceptible to microbial contamination. Pathogenic bacteria may attach themselves to device surfaces of catheters or implants by formation of chemically complex biofilms, which may be the direct cause of device failure. Extracellular bacterial lipases are particularly abundant at sites of infection. Herein it is shown how active or proactive compounds attached to polymeric surfaces using lipase-sensitive linkages, such as fatty acid esters or anhydrides, may be released in response to infection. Proof-of-concept of the responsive material is demonstrated by the bacteria-triggered release of antibiotics to control bacterial populations and signaling molecules to modulate quorum sensing. The self-regulating system provides the basis for the development of device-relevant polymeric materials, which only release antibiotics in dependency of the titer of bacteria surrounding the medical device.
Binding of Neurotransmitters to Lipid Membranes

We have performed a series of thermodynamic measurements and molecular dynamics (MD) simulations to study the interactions between the neurotransmitters (NTs) 5-hydroxytryptamine (5-HT), g-aminobutyrate (GABA), glycine (GLY), acetylcholine (ACH) and glutamate (GLU) as well as the amidated / acetylated g-aminobutyrate (GABAneu) with a dipalmitoylphosphatidylcholine (DPPC) bilayer. This study was motivated by recent research results that suggested that neural transmission may also be affected by nonspecific interactions of NTs with the lipid matrix of the synaptic membrane. Our results revealed that dependent on the nature of NTs, some of the NTs penetrate into the bilayer. We found that membrane affinity can be ranked with increasing affinity as follows: ACH ~ GLU << GABA < GLY << GABAneu << 5-HT. The latter three penetrated the bilayer at most with the deepest location being close to the glycerol backbone of the phospholipids. It is surprising that hydrophilic solutes can deeply penetrate into the membrane pointing to the fact that membrane affinity is governed by specific interactions. Our MD simulations identified the salt-bridge between the primary amine of NTs and the lipid phosphate group as the most important interaction by which the NTs are anchored to the membrane. These distinctive interactions could be related to nonspecific effects of these neurotransmitters and could point to a bilayer-mediated modulation of nerve transmission. However, due to the strong variability in affinity observed for the different NTs, this attraction is not an inherent property of all neurotransmitters.

General information

State: Published
Organisations: Department of Chemistry, Physical and Biophysical Chemistry, Department of Chemistry, Roskilde University, Technical University of Denmark
Publication date: 2014
Main Research Area: Technical/natural sciences

Publication information
Biocatalytic production of 3′-sialyllactose by use of a modified sialidase with superior trans-sialidase activity

Casein glycomacropeptide (cGMP) and lactose, which are purified (or semi-purified) components obtained from side streams from dairy industry operations, were used as substrates for enzyme catalyzed production of 3′-sialyllactose, a model case compound for human milk oligosaccharides (HMOs). The enzyme employed was a mutated sialidase, Tr6, derived from Trypanosoma rangeli, and expressed in Pichia pastoris after codon-optimization. The Tr6 contained 6 point mutations and exhibited trans-sialidase activity. The Tr6 trans-sialidase reaction conditions were tuned for maximizing Tr6 catalyzed 3′-sialyllactose production by optimizing pH, temperature, acceptor, and donor concentrations using response surface designs. At the optimum reaction conditions, the Tr6 catalyzed the transfer of sialic acid from cGMP to lactose at high efficiency without substantial hydrolysis of the 3′-sialyllactose product. The robustness of the Tr6 catalyzed reaction was verified at 5L-scale providing a yield of 3.6g 3′-sialyllactose at an estimated molar trans-sialylation yield of 50% on the 3′-sialyl in cGMP. Lacto-N-tetraose and lacto-N-fucopentaoses also functioned as acceptor molecules demonstrating the versatility of the Tr6 trans-sialidase for catalyzing sialyl-transfer for generating different HMOs. The data signify the applicability of enzymatic trans-sialylation on dairy side-stream components for production of human milk oligosaccharides.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, Organic Chemistry, Department of Chemistry, Department of Systems Biology, University of Southern Denmark
Pages: 265-270
Publication date: 2014
Main Research Area: Technical/natural sciences

Publication information
Journal: Process Biochemistry
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ISSN (Print): 1359-5113
Ratings:
  BFI (2018): BFI-level 1
  Web of Science (2018): Indexed yes
  BFI (2017): BFI-level 1
  Web of Science (2017): Indexed Yes
  BFI (2016): BFI-level 1
  Scopus rating (2016): SJR 0.819 SNIP 1.075 CiteScore 2.87
  Web of Science (2016): Indexed yes
  BFI (2015): BFI-level 1
  Scopus rating (2015): SJR 0.923 SNIP 1.234 CiteScore 3.01
  Web of Science (2015): Indexed yes
  BFI (2014): BFI-level 1
  Scopus rating (2014): SJR 0.989 SNIP 1.438 CiteScore 3.05
  Web of Science (2014): Indexed yes
  BFI (2013): BFI-level 1
  Scopus rating (2013): SJR 0.994 SNIP 1.493 CiteScore 3.06
  ISI indexed (2013): ISI indexed yes
  Web of Science (2013): Indexed yes
Catalytic Deoxygenation of Renewable Chemicals – Structure-Performance Studies

Generation of chemicals from a viable feedstock is an increasingly interesting field. One of the major issues is the high oxygen ratios in biomass. There are a multitude of ways to remove oxygen from organic molecules. This thesis deals with two topics: The dehydration of glucose into HMF and the decarbonylation of aldehydes both heterogeneous and in ionic liquids.

Chapter 1 provides a walkthrough of areas such as green chemistry, ionic liquids, biomass, dehydration of glucose in ionic liquids and decarbonylation. The topics are all taking into account the current research and is subjectively chosen to provide a broad platform for the following chapters. Furthermore, the objectives for the thesis are listed here.

Chapter 2 deals with the synthetic preparation of the catalysts and the catalytic setups.

Chapter 3 deals with the dehydration of glucose into HMF in ionic liquids. The system was investigated thoroughly via several spectroscopic techniques. This was done in order to obtain novel information in regard to the catalytically active sites. EXAFS results showed that during the catalytic reaction, a species of the form CrCl4O2 was formed from CrCl6 in the solution. These are the predominant chromium containing species in the solution. EPR results showed the presence of a $S=1/2$ spin system, and the only possible choice is radical formation. Optical absorption spectroscopy showed a change in the ligand field around the chromium.

Chapter 3 also deals with the homogeneous decarbonylation of aldehydes. The investigation of the effects of the ionic liquids in the catalytically active species is investigated in depth and the system [Rh(dppp)2]Cl in BMImCl was shown to be the most active combination. The reusability of the system showed great potential. The system showed a potential to decarbonylate both aliphatic and aromatic aldehydes.

Finally Chapter 3 looks at the heterogeneous decarbonylation of aldehydes, focussing on a continuous flow setup. The
catalytic effect of oxidation state and ligandsphere is investigated. And the effects of temperature, solvent and substrate were under scrutiny. The catalyst decomposition was pictured by the aid of TEM and the formation of nanoparticles explained.

Chapter 4 concerns the summation of the results as well as the future perspectives for the respective applications and scientific developments.

**General information**
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Authors: Malcho, P. (Intern), Riisager, A. (Intern)
Number of pages: 154
Publication date: 2014

**Publication information**
Publisher: Technical University of Denmark, Department of Chemical Engineering
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
Catalytic Deoxygenation of Renewable Chemicals..PDF
Publication: Research › Ph.D. thesis – Annual report year: 2014

**Catalytic routes from biomass to fuels**
The carbon-based chemicals and fuels that are necessary to meet the energy demand for our society originate presently almost exclusively from inexpensive fossil resources – coal, oil and natural gas. The forecast of diminishing and more expensive petroleum reserves has, however, engaged the chemical industry to find new feasible chemocatalytic routes to convert the components of lignocellulosic plant biomass (green biomass) as well as aquatic biomass (blue biomass) into potential platform chemicals that can replace the fossil based chemicals in order to leave the chemical supply and value chain unaffected. This presentation will survey the status of biofuels production from different sources, and discuss the sustainability of making transportation fuels from biomass. Furthermore, recently developed chemocatalytic technologies that allow efficient conversion of lignocellulosic biomass components into transportation fuels and fuel additives will be highlighted.

**General information**
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Authors: Riisager, A. (Intern)
Number of pages: 1
Publication date: 2014

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Title of host publication: Abstract Book - DTU Sustain Conference 2014
Place of publication: Kgs. Lyngby
Publisher: Technical University of Denmark (DTU)
Main Research Area: Technical/natural sciences
Conference: DTU Sustain Conference 2014, Lyngby, Denmark, 17/12/2014 - 17/12/2014
Publication: Research - peer-review › Conference abstract in proceedings – Annual report year: 2014

**Catalytic Synthesis of Nitriles in Continuous Flow**
The objective of this thesis is to report the development of a new, alternative process for the flexible production of nitrile compounds in continuous flow. Nitriles are an important class of compounds that find applications as solvents, chemical intermediates and pharmaceutical compounds. The process reported here involves the oxidative dehydrogenation of amine compounds to their corresponding nitrile using air as the oxidant, water as the solvent where possible and solid RuO₂/Al₂O₃ catalysts.Chapter 1 beings by outlining the aims of this thesis and then gives a short, basic introduction to concepts and techniques that are important to the contents of this thesis. Furthermore, relevant literature is reviewed to support the choice of using RuO₂/Al₂O₃ catalysts and the oxidative dehydrogenation of amines for the desired new process for the production of nitriles.Chapter 2 describes a new, alternative path to acetonitrile from ethanol via the oxidative dehydrogenation of ethylamine. The catalytic activity and product ratios of the batch and continuous flow reactions are compared and the effect of reaction conditions on the reaction is investigated. The effects of ammonia in the reaction and of catalyst calcination are also explored. High conversions (up to 100 %) and selectivities (80-90 %) are reported using optimized reaction conditions.Chapter 3 includes details of in situ infrared spectroscopy experiments, observing the surface of the RuO₂/Al₂O₃ catalyst during calcination in air, oxidative dehydrogenation of ethylamine and post-reaction purging.Chapter 4 Outlines the application of RuO₂/Al₂O₃ catalysts to the oxidative dehydrogenation of benzylamine in air, utilizing a new reaction setup. Again, batch and continuous flow reactions are compared and the effects of reaction conditions, ammonia presence and catalyst calcination are reported. Moderate benzonitrile yields (up to 62 %) and high conversions (up to 100 %) are reported.Chapter 5 describes the detailed characterization of RuO₂/Al₂O₃ catalysts and optimization of the catalyst ruthenium loading. Application of optimized RuO₂/Al₂O₃ catalysts to the
oxidative dehydrogenation of benzylamine is described and increased benzonitrile yields are reported (up to 82%). Chapter 6 reports the application of oxidative dehydrogenation of amines using air and RuO$_2$/Al$_2$O$_3$ catalysts to a range of substituted aromatic amines and longer chain aliphatic amines. Substituent groups of aromatic amines are found to effect both the rate of amine conversion and nitrile production. Novel attempts are made to apply the Hammett relationship to the oxidative dehydrogenation of amines using air and RuO$_2$/Al$_2$O$_3$ catalysts in continuous flow. The effect of the presence of water in the reaction is also investigated. Chapter 7 includes an overview of how the contents of this thesis attempt to cover the aims stated in Chapter 1 and suggests future improvements to be made to the nitrile production process.

**General information**
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry
Authors: Nordvang, E. C. (Intern), Fehrmann, R. (Intern), Riisager, A. (Intern)
Number of pages: 176
Publication date: 2014

**Characterization of an Alkali- and Halide-Resistant Laccase Expressed in E. coli: CotA from Bacillus clausii**
The limitations of fungal laccases at higher pH and salt concentrations have intensified the search for new extremophilic bacterial laccases. We report the cloning, expression, and characterization of the bacterial cotA from Bacillus clausii, a supposed alkalophilic ortholog of cotA from B. subtilis. Both laccases were expressed in E. coli strain BL21(DE3) and characterized fully in parallel for strict benchmarking. We report activity on ABTS, SGZ, DMP, caffeic acid, promazine, phenyl hydrazine, tannic acid, and bilirubin at variable pH. Whereas ABTS, promazine, and phenyl hydrazine activities vs. pH were similar, the activity of B. clausii cotA was shifted upwards by 0.5–2 pH units for the simple phenolic substrates DMP, SGZ, and caffeic acid. This shift is not due to substrate affinity (KM) but to pH dependence of catalytic turnover: The kcat of B. clausii cotA was 1 s$^{-1}$ at pH 6 and 5 s$^{-1}$ at pH 8 in contrast to 6 s$^{-1}$ at pH 6 and 2 s$^{-1}$ at pH 8 for B. subtilis cotA. Overall, kcat/KM was 10-fold higher for B. subtilis cotA at pHopt. While both proteins were heat activated, activation increased with pH and was larger in cotA from B. clausii. NaCl inhibited activity at acidic pH, but not up to 500–700 mM NaCl in alkaline pH, a further advantage of the alkali regime in laccase applications. The B. clausii cotA had a 20 minutes half-life at 80°C, less than the 50 minutes at 80°C for cotA from B. subtilis. While cotA from B. subtilis had optimal stability at pH 8, the cotA from B. clausii displayed higher combined salt- and alkali-resistance. This resistance is possibly caused by two substitutions (S427Q and V110E) that could repel anions to reduce anion-copper interactions at the expense of catalytic proficiency, a trade-off of potential relevance to laccase optimization.

**General information**
State: Published
Organisations: Department of Chemistry, Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, Physical and Biophysical Chemistry
Authors: Brander, S. (Intern), Mikkelsen, J. D. (Intern), Kepp, K. P. (Intern)
Number of pages: 11
Publication date: 2014
Main Research Area: Technical/natural sciences
Characterization of novel thermostable bacterial Laccase-like multi-copper oxidases

Laccase-like Multi-copper Oxidases (LMCOs) catalyze the oxidation of a broad range of substrates in a redox reaction coupled to the complete reduction of molecular oxygen to water. The reaction is catalyzed by four coupled copper-ions that are positioned in the LMCO in such a way, that the substrate bind to one side of the enzyme, while oxygen is recruited and water expelled on the other. This powerful mechanism makes LMCOs clean enzyme substitutions in all chemical processes that are traditionally driven by the addition of reactive oxygen species such as hydrogen peroxide. E.g. dye decolorization, bleaching of paper pulp, delignification of biomass and remediation of polluted water. In order to widen the applicability of LMCOs, it is important to establish the properties and substrate specificities of naturally occurring LMCOs. This is especially true for LMCOs from bacteria, whose role in nature is not well understood. If we want to change a LMCO, to specifically catalyze a man-made reaction, it becomes important to have a diverse and stable starting protein. In this regard bacterial LMCOs are of special interest, because they are intrinsically thermostable and distinct variants can be found in the rapidly increasing number of sequenced bacterial genomes. This dissertation describes our effort to identify and express novel LMCOs from bacterial origins. Some of these enzymes were also characterized, and special emphasis was put on revealing their substrate specificity and thermostability. Bacillus clausii KSM-16 is known to produce a potent alkalophilic and thermostable protease that is sometimes used in laundry detergent mixes. We have expressed and characterized the LMCO coded in the genome of the same bacterial strain, and found that it is a thermostable enzyme
with substrate specificity similar to that of the well-characterized Bacillus subtilis CotA. Stability and catalytic reactivity were both slightly less than B. subtilis CotA, while the preferred pHs for both properties were shifted about 1 unit to the more alkaline. Thermobaculum terrenum is a thermophilic bacterium cultured from a hot dirt patch in Yellowstone National Park. It belongs to the evolutionary interesting phylum Chloroflexi that has been proposed to represent some of the earliest lifeforms on Earth. The genome of T. terrenum codes for a LMCO, and we have expressed and characterized the enzyme. It is the second most thermostable characterized LMCO, but was only able to selectively oxidize two out of 57 tested substrates. Of special interest to the characterization of bacterial LMCOs is the thermostability. Measurement of thermal inactivation of LMCOs is hampered by an often observed heat-induced increase in enzyme activity. We found that heat activation is accompanied by a change in the Electron Paramagnetic Spectroscopy (EPR) spectrum, and used this to characterize the mechanism behind the process. It is a redox transformation, and for the T. terrenum LMCO it was found to be controlled by temperature and NaCl, while the similar transformation in B. subtilis CotA also needed the reducing agent, ascorbate, in order to take place. The discovered mechanism can most likely be expanded to also encompass other LMCOs that have previously been shown to undergo heat-activation.

**General information**
State: Published
Organisations: Department of Chemistry, Center for BioProcess Engineering, Physical and Biophysical Chemistry, Department of Chemical and Biochemical Engineering
Authors: Brander, S. (Intern), Kepp, K. P. (Intern), Mikkelsen, J. D. (Intern)
Number of pages: 127
Publication date: 2014

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Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
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Source: PublicationPreSubmission
Source-ID: 105599039
Publication: Research › Ph.D. thesis – Annual report year: 2015

**Chemical Production of Graphene Catalysts for Electrochemical Energy Conversion**

**General information**
State: Published
Organisations: Department of Chemistry, NanoChemistry, Organic Chemistry
Authors: Seselj, N. (Intern), Engelbrekt, C. (Intern), Ulstrup, J. (Intern), Zhang, J. (Intern)
Number of pages: 1
Publication date: 2014
Main Research Area: Technical/natural sciences
Electronic versions:
Source: PublicationPreSubmission
Source-ID: 120486338
Publication: Research - peer-review › Poster – Annual report year: 2014

**Chemical tools for unraveling the substrate specificity of the lysine deacylase enzymes**
The lysine deacylase (KDAC) enzymes catalyze hydrolytic removal of acyl functionalities from the ε-amino group of lysine residues in a variety of proteins including histones, and KDAC-mediated deacetylation of proteins has been established as a key epigenetic and metabolic regulator. Recent studies have highlighted lysine acetylation as a general post-translational modification (PTM), and a growing list of non-histone proteins has been identified as substrates for the KDACs, thereby extending their potential impact on cellular function. Furthermore, other acyl groups (e.g., crotonyl, malonyl, succinyl, glutaryl, myristoyl and 3-phosphoglyceroyl) have been identified as lysine PTMs, and both zinc- and NAD+-dependent KDACs have demonstrated capability to remove such modifications. These findings suggest that KDACs with impaired deacetylase activity might in fact be functional deacylases catalyzing hydrolysis of other acylamides. To address these interesting observations, we have synthesized a library of substrates containing different peptide scaffolds functionalized with a number of N-ε-acyl moieties. Library synthesis and its evaluation against a panel of human KDACs including zinc-dependent HDACs 1–11 as well as NAD +-dependent sirtuins (SIRT1–7) will be discussed.

**General information**
State: Published
Organisations: Department of Chemistry, Organic Chemistry
Co-C Dissociation of Adenosylcobalamin (Coenzyme B-12): Role of Dispersion, Induction Effects, Solvent Polarity, and Relativistic and Thermal Corrections

Quantum-chemical cluster modeling is challenged in the limit of large, soft systems by the effects of dispersion and solvent, and well as other physical interactions. Adenosylcobalamin (AdoCbl, coenzyme B-12), as one of the most complex cofactors in life, constitutes such a challenge. The cleavage of its unique organometallic Co-C bond has inspired multiple studies of this cofactor. This paper reports the fully relaxed potential energy surface of Co-C cleavage of AdoCbl, including for the first time all side-chain interactions with the dissociating Ado group. Various methods and corrections for dispersion, relativistic effects, solvent polarity, basis set superposition error, and thermal and vibrational effects were investigated, totaling more than SSO single-point energies for the large model. The results show immense variability depending on method, including solvation, functional type, and dispersion, challenging the conceived accuracy of methods used for such systems. In particular, B3LYP-D3 seems to severely underestimate the Co-C bond strength, consistent with previous results, and BP86 remains accurate for cobalamins when dispersion interactions are accounted for.
 Combined Use of Both Experimental and Theoretical Methods in the Exploration of Reaction Mechanisms in Catalysis by Transition Metals

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry
Authors: Lupp, D. (Intern), Christensen, N. J. (Intern), Fristrup, P. (Intern)
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Main Research Area: Technical/natural sciences
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Source: PublicationPreSubmission
Source-ID: 101719319
Publication: Research - peer-review › Book chapter – Annual report year: 2014

Combining Organometallic Catalysis and Organocatalysis for the Synthesis of Heterocyclic Scaffolds
The main work presented in this thesis describes the development of efficient and novel methodologies for the synthesis of pharmaceutically interesting indole-containing alkaloids, i.e., the 1,2,3,4-tetrahydro-𝛽-carboline and the 1,2,3,4-tetrahydrocarbazole scaffolds. The synthesis of 1,2,3,4-tetrahydro-𝛽-carbolines was based on a transition metal/Brensted acid-catalyzed tandem isomerization/N-acyliminium ion cyclization of N-acylated allylic tryptamines. First, the reaction

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Source: FindIt
Source-ID: 269921886
Publication: Research - peer-review › Journal article – Annual report year: 2014
conditions for the tandem reaction were optimized to high efficiency, culminating in the use of the ruthenium hydride catalyst RuHCl(CO)(PPh3)3 combined with diphenyl phosphate at elevated temperature (refluxing toluene). The optimized reaction conditions were, in most cases, successfully applied to a broad range of Nacylated allyltryptamines, and the desired products were obtained in good yields (68–96%). With highly electron-withdrawing substituents, the reaction resulted in the formation of the corresponding enamides. When substituents capable of coordinating the catalyst were used, no conversions of the starting materials were observed. In an enantioselective version of the reaction, the substituent α to the nitrogen in the allylic system proved to be highly important for the enantioselectivity. Enantiomeric excesses up to 57% was obtained.

The synthesis of 1,2,3,4-tetrahydrocarbazole relied on novel Brønsted acidcatalyzed Friedel-Crafts-type reactions. Three different kinds of 1,2,3,4-tetrahydrocarbazole could be synthesized from one common carbonyl starting material. Type 1 reactions involved direct intramolecular cyclization from an indole moiety to an aldehyde resulting in the corresponding alcohols. The reaction was limited to electron-rich nucleophiles. Type 2 reactions deal with addition of nucleophiles, either to the cyclized alcohol obtained from type 1 reactions or directly to the carbonyl followed by cyclization. The reaction conditions were dependent on whether the addition of the nucleophile occurred before or after cyclization. An enantioselective version of the reaction was highly dependent on the substitution pattern, as enantiomeric excesses between 6 and >99% were obtained in 35–94% isolated yield. Type 3 reactions aimed for addition of organometallic reagents to the carbonyl with subsequently cyclization. No one-pot reaction directly from the carbonyl species to the 1,2,3,4-tetrahydrocarbazole was developed. A two-step synthetic route, via the alcohols, was investigated and found to be highly dependent on the presence of carbocation stabilizing groups around the alcohol; therefore only three final type 3 products were synthesized in good yields (64–95%).

A small project, which attempted to take advantage of the above described to be use as a novel cleavage strategy for solid support linkers, is also presented here. Unfortunately, no successful conditions were developed.

**General information**
State: Published
Organisations: Department of Chemistry, Organic Chemistry
Authors: Hansen, C. L. (Intern), Nielsen, T. E. (Intern), Tanner, D. A. (Intern)
Number of pages: 247
Publication date: 2014

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Place of publication: Kgs. Lyngby
Publisher: Technical University of Denmark (DTU)
Original language: English
Main Research Area: Technical/natural sciences
Publication: Research › Ph.D. thesis – Annual report year: 2015

**Comparative Systems Biology Analysis To Study the Mode of Action of the Isothiocyanate Compound Iberin on Pseudomonas aeruginosa**

Food is now recognized as a natural resource of novel antimicrobial agents, including those that target the virulence mechanisms of bacterial pathogens. Iberin, an isothiocyanate compound from horseradish, was recently identified as a quorum-sensing inhibitor (QSI) of the bacterial pathogen Pseudomonas aeruginosa. In this study, we used a comparative systems biology approach to unravel the molecular mechanisms of the effects of iberin on QS and virulence factor expression of P. aeruginosa. Our study shows that the two systems biology methods used (i.e., RNA sequencing and proteomics) complement each other and provide a thorough overview of the impact of iberin on P. aeruginosa. RNA sequencing-based transcriptomics showed that iberin inhibits the expression of the GacA-dependent small regulatory RNAs RsmY and RsmZ; this was verified by using gfp-based transcriptional reporter fusions with the rsmY or rsmZ promoter regions. Isobaric tags for relative and absolute quantitation (iTraq) proteomics showed that iberin reduces the abundance of the LadS protein, an activator of GacS. Taken together, the findings suggest that the mode of QS inhibition in iberin is through downregulation of the Gac/Rsm QS network, which in turn leads to the repression of QS-regulated virulence factors, such as pyoverdine, chitinase, and protease IV. Lastly, as expected from the observed repression of small regulatory RNA synthesis, we also show that iberin effectively reduces biofilm formation. This suggests that small regulatory RNAs might serve as potential targets in the future development of therapies against pathogens that use QS for controlling virulence factor expression and assume the biofilm mode of growth in the process of causing disease.

**General information**
State: Published
Organisations: Department of Chemistry, Organic Chemistry, Nanyang Technological University, University of Copenhagen
Number of pages: 12
Pages: 6648-6659
Publication date: 2014
Main Research Area: Technical/natural sciences
Compressibilities and viscosities of reference, vegetable, and synthetic gear lubricants

Nowadays, one of the primary choices of base oils for environmentally aware lubricants is vegetable oils. This is due to their good natural biodegradability and very low toxicity in combination with very good lubricity characteristics. The development of new vegetable-based lubricants requires the knowledge of their thermophysical properties such as their viscosity or density, among others. Regarding this issue, in this work, we have carried out density measurements between 278.15 and 398.15 K and pressures up to 120 MPa and calculated the isothermal compressibility and isobaric thermal expansivity values of six gear lubricants, two of them reference mineral oils and the other four developed biodegradable oils based in high oleic sunflower oil or in synthetic esters. It was found that all of the lubricants have both similar compressibilities and similar expansivities. Dowson and Higginson, Zhu and Wen, Jacobson and Vinet equations of state predict the experimental density values with absolute average deviations (AADs), that is, AAD % lower than 0.3, 0.4, and 0.6%, respectively, whereas Tammann-Tait and the modified Tait equations correlate these experimental densities with AAD % of 0.02 and 0.06%. Dowson and Higginson and Zhu and Wen equations of state do not predict well the isothermal compressibilities, with AAD % being around 45% for both equations. Moreover, the viscosities were measured in the temperature range from 278.15 to 373.15 K at atmospheric pressure for these oils, and the viscosity index was also determined. New formulated oils present the highest viscosity indexes and the lowest viscosity data at low temperatures; therefore, they become the most suitable for machinery cold start. © 2014 American Chemical Society.

General information
State: Published
Organisations: Center for Energy Resources Engineering, Department of Chemistry, CERE – Center for Energy, Ressources Engineering, University of Vigo, Universidad de Santiago de Compostela
Authors: Regueira Muñiz, T. (Intern), Lugo, L. (Ekstern), Fernández, J. (Ekstern)
Number of pages: 12
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BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.1 SJR 0.945 SNIP 1.139
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.949 SNIP 1.146 CiteScore 2.87
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.012 SNIP 1.292 CiteScore 2.85
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 0.982 SNIP 1.243 CiteScore 2.6
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Computational Investigation of Enthalpy-Entropy Compensation in Complexation of Glycoconjugated Bile Salts with β-Cyclodextrin and Analogs

The inclusion complexes of glycoconjugated bile salts with beta-cyclodextrin (beta-CD) and 2-hydroxypropyl-beta-cyclodextrins (HP-beta-CD) in aqueous solution were investigated by molecular dynamics simulations to provide a molecular explanation of the experimentally observed destabilizing effect of the HP substituents. Good agreement with experimental data was found with respect to penetration depths of CDs. An increased degree of HP substitution (DS) resulted in an increased probability of blocking the cavity opening, thereby hindering the bile salt from entering CD. Further, the residence time of water molecules in the cavity increased with the DS. Release of water from the cavity resulted in a positive enthalpy change, which correlates qualitatively with the experimentally determined increase in complexation enthalpy and contributes to the enthalpy-entropy compensation. The positive change in complexation entropy with DS was not able to compensate for this unfavorable change in enthalpy induced by the HP substituents, resulting in a destabilizing effect. This was found to originate from fixation of the HP substituents and decreased free rotation of the bile salts within the CD cavities.
Computing Stability Effects of Mutations in Human Superoxide Dismutase 1

Protein stability is affected in several diseases and is of substantial interest in efforts to correlate genotypes to phenotypes. Superoxide dismutase 1 (SOD1) is a suitable test case for such correlations due to its abundance, stability, available crystal structures and thermochemical data, and physiological importance. In this work, stability changes of SOD1 mutations were computed with five methods, CUPSAT, I-Mutant2.0, I-Mutant3.0, PoPMuSiC, and SDM, with emphasis on structural sensitivity as a potential issue in structure-based protein calculation. The large correlation between experimental literature data of SOD1 dimers and monomers (r = 0.82) suggests that mutations in separate protein monomers are mostly additive. PoPMuSiC was most accurate (typical MAE ∼ 1 kcal/mol, r ∼ 0.5). The relative performance of the methods was not very structure-dependent, and the more accurate methods also displayed less structural sensitivity, with the standard deviation from different high-resolution structures down to ∼0.2 kcal/mol. Structures of variable resolution and number of protein copies locally affected specific sites, emphasizing the use of state-relevant crystal structures when such sites are of interest, but had little impact on overall batch estimates. Protein-interaction effects (as a mimic of crystal packing) were small for the more accurate methods. Thus, batch computations, relevant to, e.g., comparisons of disease/nondisease mutant sets or different clades in phylogenetic trees, are much more significant than single mutant calculations and may be the only meaningful way to computationally bridge the genotype–phenotype gap of proteomics. Finally, mutations involving glycine were most difficult to model, of relevance to future method improvement. This could be due to structure changes (glycine has a low structural propensity) or water colocalization with glycine.

General information
State: Published
Organisations: Department of Chemistry, Physical and Biophysical Chemistry
Authors: Kepp, K. P. (Intern)
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Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.03 SJR 1.348 SNIP 1.02
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.367 SNIP 1.096 CiteScore 3.25
Web of Science (2015): Indexed yes
Contact Resistance of Tantalum Coatings in Fuel Cells and Electrolyzers using Acidic Electrolytes at Elevated Temperatures

Tantalum has so far been found to be the only construction material with sufficient corrosion resistance for high temperature polymer electrolyte membrane electrolyzers using acidic electrolytes above 100°C. In this work the interfacial contact resistances of tantalum plates and tantalum coated stainless steel were found to be far below the US Department of Energy target value of 10mcm². The
good contact resistance of tantalum was demonstrated by simulating high temperature polymer electrolyte membrane electrolysis conditions by anodization performed in 85% phosphoric acid at 130°C, followed by contact resistance measurements. Upon anodization the contact resistances remained unchanged.
Controlling the stereochemistry and regularity of butanethiol self-assembled monolayers on Au(111)

The rich stereochemistry of the self-assembled monolayers (SAMs) of four butanethiols on Au(111) is described, the SAMs containing up to 12 individual C, S, or Au chiral centers per surface unit cell. This is facilitated by synthesis of enantiomerically pure 2-butanethiol (the smallest unsubstituted chiral alkanethiol), followed by in situ scanning tunneling microscopy (STM) imaging combined with density functional theory molecular dynamics STM image simulations. Even though butanethiol SAMs manifest strong headgroup interactions, steric interactions are shown to dominate SAM structure and chirality. Indeed, steric interactions are shown to dictate the nature of the headgroup itself, whether it takes on the adatom-bound motif RS•Au(0)S•R or involves direct binding of RS• to face-centered-cubic or hexagonal-close-packed sites. Binding as RS• produces large, organizationally chiral domains even when R is achiral, while adatom binding leads to rectangular plane groups that suppress long-range expression of chirality. Binding as RS• also inhibits the pitting intrinsically associated with adatom binding, desirably producing more regularly structured SAMs.

General information
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Organisations: Department of Chemistry, Organic Chemistry, NanoChemistry, Xiamen University, University of Sydney, Shanghai University
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Main Research Area: Technical/natural sciences

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Scopus rating (2016): CiteScore 13.18 SJR 7.368 SNIP 2.584
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 6.826 SNIP 2.632 CiteScore 12.81
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 6.273 SNIP 2.578 CiteScore 11.92
Web of Science (2014): Indexed yes
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Scopus rating (2013): SJR 5.953 SNIP 2.455 CiteScore 11.38
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Conversion of carbohydrates to levulinic acid esters
The present invention relates to the field of converting carbohydrates into levulinic acid, a platform chemical for many chemical end products. More specifically the invention relates to a method for converting carbohydrates such as mono-, di- or polysaccharides, obtained from for example biomass production into a suitable levulinic acid ester in the presence of a zeolite or zeotype catalyst and a suitable alcohol, and the ester may be further converted into levulinic acid if desired.

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Authors: Shunmugavel, S. (Intern), Riisager, A. (Intern)
Publication date: 2014

Publication information
Coordination Environment of Copper Sites in Cu-CHA Zeolite Investigated by Electron Paramagnetic Resonance

Cu-CHA combines high activity for the selective catalytic reduction (SCR) reaction with better hydrothermal stability and selectivity compared to other copper-substituted zeolites. At the same time Cu-CHA offers an opportunity for unraveling the coordination environment of the copper centers since the zeolite framework is very simple with only one crystallographically independent tetrahedral site (T-site). In this study the results of an X-band electron paramagnetic resonance (EPR) investigation of ion-exchanged Cu-CHA zeolite with a Si/Al ratio of 14 ± 1 is presented. Different dehydration treatments and rehydration experiments are performed in situ while monitoring with EPR. The results are compared with recent literature evidence from temperature-programmed reduction, X-ray methods, IR spectroscopic methods, and UV–visible spectroscopy. On the basis of these findings quantitative information is obtained for the different copper positions in dehydrated Cu-CHA. The well-defined copper sites in the six-membered ring of the CHA structure are found to be EPR active, to give two distinct sets of signals in an approximate 1:1 ratio, and to add up to 19 ± 2% of the total copper in the material. The long-standing question of the EPR silent monomeric Cu2+ in copper-substituted zeolites is suggested to be copper species with an approximate trigonal coordination sphere appearing during the dehydration. After complete dehydration at 250 °C the majority of the EPR silent Cu2+ is suggested to exist as Cu2+–OH– coordinated to two framework oxygen atoms located in the microenvironment of an isolated Al T-site.
The purpose of this PhD project was to develop an enantioselective cobalt-mediated radiofluorination of epoxides and apply this methodology for radiosynthesis of the PET radiopharmaceutical [18F]FMISO. The developed procedure utilizes [18F]HF-gas (as an efficient source of nucleophilic 18F-fluoride) in a combination with chiral base ((-)tetramisole), chiral Lewis acid ((R,R)-Co(salen)) and hexafluoroisopropanol, providing the corresponding (S)-[18F]fluorohydrides enantioselectively (20-46% enantiomeric excess) with high yields (78-93 % radiochemical yield). The enantioselective Co(salen)-mediated no-carrier-added radiofluorination of epoxides has been achieved for the first time. A number of model meso-epoxides were successfully radiofluorinated producing 18F-fluorohydrines in high RCC and RCY, and modest enantioselectivity. The developed procedure is simple, rapid and lends itself to easy automation. This methodology was adopted for the first automated enantioselective single step radiosynthesis of PET hypoxia radiotracer [18F]FMISO in 81% RCY and 55% enantioselectivity. The use of enantiopure substrates for the synthesis of both enantiomers allowed us to obtain the (S) and (R)-[18F]FMISO enantiomers with > 99% enantiopurity. In vivo quantitative and pharmacokinetic data were obtained for the first time for the both enantiomers of [18F]FMISO. The R-form showed higher uptake in tumor as well as in muscle tissues, thus displaying nearly identical tumor-to muscle ratios and showing very similar imaging profiles of both the (S) and the (R)-[18F]FMISO enantiomers.
CO₂ sorption by supported amino acid ionic liquids
The present invention concerns the absorption and desorption behaviour of carbon dioxide (CO₂) using ionic liquids derived from amino acids adsorbed on porous carrier materials.

Critical V₂O₅/TeO₂ ratio inducing abrupt property changes in vanadium tellurite glasses
Transition metal containing glasses have unique electrical properties and are therefore often used for electrochemical applications, such as in batteries. Among oxide glasses, vanadium tellurite glasses exhibit the highest electronic conductivity and thus the high potential for applications. In this work, we investigate how the dynamic and physical properties vary with composition in the vanadium tellurite system. The results show that there exists a critical V₂O₅ concentration of 45 mol %, above which the local structure is subjected to a drastic change with increasing V₂O₅, leading to abrupt changes in both hardness and liquid fragility. Electronic conductivity does not follow the expected correlation to the valence state of the vanadium as predicted by the Mott-Austin equation but shows a linear correlation to the mean distance between vanadium ions. These findings could contribute to designing optimum vanadium tellurite compositions for electrochemical devices. The work gives insight into the mechanism of electron conduction in the vanadium tellurite systems. (Graph Presented).
Original language: English

Electric conductivity, Glass, Tellurium compounds, Transition metals, Electrochemical applications, Electrochemical devices, Electron conduction, Electronic conductivity, Linear correlation, Liquid fragilities, Property changes, Vanadium tellurite, Vanadium
Crossflow and water banks in viscous dominant regimes of waterflooding

Understanding the crossflow in multilayered reservoirs is of great importance for designing mobility control methods for enhanced oil recovery. The authors reveal saturation profiles in stratified reservoirs to study the interlayer communication in the viscous dominant regime. The displacement profiles are more even and smoother in a communicating layer-cake reservoir than in a noncommunicating one. Water banks and transition zones may be observed. Analysis indicates that the phenomena are attributed to the enhanced crossflow due to large mobility ratios (water-oil). The mobility control techniques that take advantage of crossflow between layers may be more efficient with large mobility ratios. © 2014 Copyright Taylor & Francis Group, LLC.
Depolymerization of organosolv lignin using doped porous metal oxides in supercritical methanol

An isolated, solvent-extracted lignin from candlenut (Aleurites moluccana) biomass was subjected to catalytic depolymerization in the presence of supercritical methanol, using a range of porous metal oxides derived from hydrotalcite-like precursors. The most effective catalysts in terms of lignin conversion to methanol-soluble products, without char formation, were based on copper in combination with other dopants based on relatively earth-abundant metals. Nearly complete conversion of lignin to bio-oil composed of monomers and low-mass oligomers with high aromatic content was obtained in 6 h at 310 °C using a catalyst based on a Cu- and La-doped hydrotalcite-like precursor. Product mixtures were characterized by NMR spectroscopy, gel permeation chromatography, and GC-MS. © 2014.

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Yale University
Authors: Warner, G. (Ekstern), Hansen, T. S. (Intern), Riisager, A. (Intern), Beach, E. S. (Ekstern), Barta, K. (Ekstern), Anastas, P. T. (Ekstern)
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Scopus rating (2015): SJR 2.255 SNIP 1.908 CiteScore 5.47
Web of Science (2015): Indexed yes
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Scopus rating (2014): SJR 2.41 SNIP 2.104 CiteScore 5.3
Dereplication Guided Discovery of Secondary Metabolites of Mixed Biosynthetic Origin from Aspergillus aculeatus

Investigation of the chemical profile of the industrially important black filamentous fungus Aspergillus aculeatus by UHPLC-DAD-HRMS and subsequent dereplication has led to the discovery of several novel compounds. Isolation and extensive 1D and 2D NMR spectroscopic analyses allowed for structural elucidation of a dioxomorpholine, a unique okaramine, an aflavinine and three novel structures of mixed biosynthetic origin, which we have named aculenes A-C. Moreover, known analogues of calbistrins, okaramines and secalonic acids were detected. All novel compounds were tested for antifungal activity against Candida albicans, however all showed only weak or no activity. Aspergillus aculeatus IBT 21030 was additionally shown to be capable of producing sclerotia. Examination of the sclerotia revealed a highly regulated production of metabolites in these morphological structures.

General information
Design, calibration and application of broad-range optical nanosensors for determining intracellular pH.

Particle-based nanosensors offer a tool for determining the pH in the endosomal-lysosomal system of living cells. Measurements providing absolute values of pH have so far been restricted by the limited sensitivity range of nanosensors, calibration challenges and the complexity of image analysis. This protocol describes the design and application of a polyacrylamide-based nanosensor (~60 nm) that covalently incorporates two pH-sensitive fluorophores, fluorescein (FS) and Oregon Green (OG), to broaden the sensitivity range of the sensor (pH 3.1-7.0), and uses the pH-insensitive fluorophore rhodamine as a reference fluorophore. The nanosensors are spontaneously taken up via endocytosis and directed to the lysosomes where dynamic changes in pH can be measured with live-cell confocal microscopy. The most important focus areas of the protocol are the choice of pH-sensitive fluorophores, the design of calibration buffers, the determination of the effective range and especially the description of how to critically evaluate results. The entire procedure typically takes 2-3 weeks.
Design, synthesis, and characterization of biomimetic oligomers

Peptides and proteins made from the 20 canonical amino acids are responsible for many processes necessary for organisms to function. Beside their composition, proteins obtain their activity and unique selectivity through an ability to display functionalities accurately in the three-dimensional space. These properties are highly sought after in pharmaceutical agents, where the interest in this class of compounds is increasing. However, due to susceptibility to proteolytic degradation in cellular environments and often poor cell-penetrating properties, this class of compounds has traditionally been considered unsuitable for drug discovery. Circumventing the inherent stability problems, non-natural peptide analogues have shown significant potential for the development of new materials and pharmacologically active ligands. Mimics of natural amino acids have received considerable attention, for their ability to mimic the structural elements seen in proteins. Two prominent peptidomimetics are ß-peptides and a-peptoids (N-alkylglycines), which have been shown to fold into helical and sheet-like arrangements. To expand the chemical space available for mimicking protein structure their features have been combined to give the ß-peptoids, which has found use in biologically active compounds but has been sparsely studied with respect to folding propensity. Thus, an aim of this Ph.D. project has been to investigate the effect of structural variations, including side chain substitution, introduction of thioamides, and trifluoroacetylation, on the cis-trans amide bond rotamer equilibria in monomer model systems. The latter systems revealed an increase in the preference for cis-amides as compared to their parent compounds and thus provide novel strategies for affecting the folding of peptoid constructs. Using NMR spectroscopy, X-ray crystallographic analysis, and density functional theory (DFT) calculations, we found evidence for the presence of thioamide–aromatic interactions through Csp2-H···Samide hydrogen bonding. Based on these studies we designed a ß-peptoid oligomer from residues prone to fit a helical arrangement found by DFT calculations. The designed oligomer indeed proved the existence of a ß-peptoid helical conformation by X-ray. Further studies of these compounds indicated a structured display in solution. These helices thus definitively show that the ß-peptoids should be considered a valid addition to the already existing ensemble of foldamer designs.

Sequences of alternating a-peptides and ß-peptoids, containing basic a-amino acid residues have been shown to possess antimicrobial activity. Using X-ray surface scattering techniques the interaction of two oligomers, containing different basic moieties, and model lipid membranes of Gram-positive and Gram-negative bacteria, respectively, were investigated. We also synthesized fluorophore labeled analogues of the hybrid oligomers, which during a preliminary biological screening, showed cases of enhanced antimicrobial activity. The X-ray scattering studies confirmed earlier findings, showing that the guanidino-group binds more deeply into the membranes of Gram-positive bacteria, and that the nitrobenzoxadiazole-fluorphore enhanced this interaction.

General information

State: Published
Organisations: Department of Chemistry
Authors: Laursen, J. S. (Intern), Olsen, C. A. (Intern)
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Publication date: 2014
Determination of iron by Z-GFAAS and the influence of short-term precision and long-term precision

A detailed method validation of graphite-furnace atomic absorption spectrometry (GFAAS) with Zeeman background correction was performed. The aim is to perform a detailed investigation of short-term precision as opposed to long-term precision. It was suggested that release of graphite flakes into the light path during measurement significantly influenced the performance of the method. It was found that significant deviations with respect to the certified values were frequent and an estimate of reliable uncertainties was obtained only after a high number of repetitions. Uncertainty of intralaboratory testing was evaluated as a method to estimate uncertainties that are comparable to uncertainties that were obtained by intralaboratory testing and to uncertainties predicted by the Horwitz curve. To a large extent, the uncertainty in measurement that was predicted by pooled calibrations corresponded to the uncertainties that were obtained from multiple determinations of unknowns. It was thus proposed that a large proportion of the difference in uncertainty in measurement between laboratories could be explained by properties of the different detectors. In order to support accuracy, it is suggested that a higher level of uncertainty should be accepted in analytical investigations.
Determination of stability constants of tauro- and glyco-conjugated bile salts with the negatively charged sulfobutylether-β-cyclodextrin: comparison of affinity capillary electrophoresis and isothermal titration calorimetry and thermodynamic analysis of the interaction

The aim of the present work was to investigate the interaction between bile salts present in the intestine of man, dog and rat with the negatively charged cyclodextrin (CD), sulfobutylether-β-cyclodextrin (SBEβCD). The interactions between bile salts and CDs are of importance for the release of CD-complexed drugs upon oral administration. This makes a good understanding of this particular interaction important for rational drug formulation. SBEβCD is a modified CD, which has attracted particular interest in formulation science. It is unique in the sense that it carries approximately seven negatively charged side chains, which can potentially interact electrostatically with the guest molecule. Bile salts are negatively charged at physiological pH, and the concomitant repulsion from SBEβCD could potentially reduce their affinity for this CD and hence their ability to expel drugs delivered as SBEβCD complexes. However, this study has demonstrated that the interaction, between a bile salts and SBEβCD is only slightly weaker than the corresponding interactions with natural βCD. Significant differences between the thermodynamics of bile salt complexes with respectively HPβCD and SBEβCD were found, when comparing the same degree of substitution. This underscores the importance of the substituents on the interactions of modified CDs with bile salts.

General information
State: Published
Organisations: Department of Chemistry, Physical and Biophysical Chemistry, H. Lundbeck A/S, Roskilde University, University of Copenhagen
Authors: Holm, R. (Forskerdatabase), Østergaard, J. (Forskerdatabase), Schönbeck, J. C. S. (Forskerdatabase), Jensen, H. (Ekstern), Shi, W. (Forskerdatabase), Peters, G. H. (Intern), Westh, P. (Ekstern)
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Scopus rating (2016): SJR 0.34 SNIP 0.484 CiteScore 1.09
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Scopus rating (2015): SJR 0.314 SNIP 0.57 CiteScore 1.32
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.455 SNIP 0.72 CiteScore 1.45
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.445 SNIP 0.6 CiteScore 1.37
ISI indexed (2013): ISI indexed no
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.521 SNIP 0.746 CiteScore 1.45
ISI indexed (2012): ISI indexed no
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.536 SNIP 0.856 CiteScore 1.88
ISI indexed (2011): ISI indexed no
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.41 SNIP 0.614
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.553 SNIP 0.679
BFI (2008): BFI-level 1
Direct catalytic transformation of carbohydrates into 5-ethoxymethylfurfural with acid–base bifunctional hybrid nanospheres

A series of acid–base bifunctional hybrid nanospheres prepared from the self-assembly of basic amino acids and phosphotungstic acid (HPA) with different molar ratios were employed as efficient and recyclable catalysts for synthesis of liquid biofuel 5-ethoxymethylfurfural (EMF) from various carbohydrates. A high EMF yield of 76.6%, 58.5%, 42.4%, and 36.5% could be achieved, when fructose, inulin, sorbose, and sucrose were used as starting materials, respectively. Although, the acid–base bifunctional nanocatalysts were inert for synthesis of EMF from glucose based carbohydrates, ethyl glucopyranoside in good yields could be obtained from glucose in ethanol. Moreover, the nanocatalyst functionalized with acid and basic sites was able to be reused several times with no significant loss in catalytic activity.
Direct Dynamics Studies of a Binuclear Metal Complex in Solution: The Interplay Between Vibrational Relaxation, Coherence, and Solvent Effects

By using a newly implemented QM/MM multiscale MD method to simulate the excited state dynamics of the Ir2(dimen)42+ (dimen = 1,8-diisocyano-p-menthane) complex, we not only report on results that support the two experimentally observed coherent dynamical modes in the molecule but also reveal a third mode, not distinguishable by spectroscopic methods. We directly follow the channels of energy dissipation to the solvent and report that the main cause for coherence decay is the initial wide range of configurations in the excited state population. We observe that the solvent can actually extend the coherence lifetime by blocking channels for intramolecular vibrational energy redistribution (IVR).

General information
State: Published
Organisations: Center for Atomic-scale Materials Design, Department of Chemistry, Physical and Biophysical Chemistry, Department of Physics, NanoChemistry, Neutrons and X-rays for Materials Physics
Authors: Dohn, A. O. (Intern), Jónsson, E. Ö. (Intern), Kjær, K. S. (Intern), Brandt van Driel, T. (Intern), Nielsen, M. M. (Intern), Jacobsen, K. W. (Intern), Henriksen, N. E. (Intern), Møller, K. B. (Intern)
Pages: 2414-2418
Publication date: 2014
Main Research Area: Technical/natural sciences
Directed Energy Transfer in Films of CdSe Quantum Dots: Beyond the Point Dipole Approximation.
Understanding of Förster resonance energy transfer (FRET) in thin films composed of quantum dots (QDs) is of fundamental and technological significance in optimal design of QD based optoelectronic devices. The separation between QDs in the densely packed films is usually smaller than the size of QDs, so that the simple point-dipole approximation, widely used in the conventional approach, can no longer offer quantitative description of the FRET dynamics in such systems. Here, we report the investigations of the FRET dynamics in densely packed films composed of multisized CdSe QDs using ultrafast transient absorption spectroscopy and theoretical modeling. Pairwise interdot transfer
time was determined in the range of 1.5 to 2 ns by spectral analyses which enable separation of the FRET contribution from intrinsic exciton decay. A rational model is suggested by taking into account the distribution of the electronic transition densities in the dots and using the film morphology revealed by AFM images. The FRET dynamics predicted by the model are in good quantitative agreement with experimental observations without adjustable parameters. Finally, we use our theoretical model to calculate dynamics of directed energy transfer in ordered multilayer QD films, which we also observe experimentally. The Monte Carlo simulations reveal that three ideal QD monolayers can provide exciton funneling efficiency above 80% from the most distant layer. Thereby, utilization of directed energy transfer can significantly improve light harvesting efficiency of QD devices.
Direct measurement of colloidal interactions between polyaniline surfaces in a uv-curable coating formulation: the effect of surface hydrophilicity/ hydrophobicity and resin composition

The interactions between polyaniline particles and polyaniline surfaces in polyester acrylate resin mixed with 1,6-hexanediol diacrylate monomer have been investigated using contact angle measurements and the atomic force microscopy colloidal probe technique. Polyaniline with different characteristics (hydrophilic and hydrophobic) were synthesized directly on spherical polystyrene particles of 10 μm in diameter. Surface forces were measured between core/shell structured polystyrene/polyaniline particles (and a pure polystyrene particle as reference) mounted on an atomic force microscope cantilever and a pressed pellet of either hydrophilic or hydrophobic polyaniline powders, in resins of various polymer:monomer ratios. A short-range purely repulsive interaction was observed between hydrophilic polyaniline (doped with phosphoric acid) surfaces in polyester acrylate resin. In contrast, interactions between hydrophobic polyaniline (doped with n-decyl phosphonic acid) were dominated by attractive forces, suggesting less compatibility and higher tendency for aggregation of these particles in liquid polyester acrylate compared to hydrophilic polyaniline. Both observations are in agreement with the conclusions from the interfacial energy studies performed by contact angle measurements.
Distinct substrate specificities of three glycoside hydrolase family 42 β-galactosidases from Bifidobacterium longum subsp. infantis ATCC 15697

Glycoside hydrolase family 42 (GH42) includes β-galactosidases catalyzing the release of galactose (Gal) from the non-reducing end of different β-d-galactosides. Health-promoting probiotic bifidobacteria, which are important members of the human gastrointestinal tract microbiota, produce GH42 enzymes enabling utilization of β-galactosides exerting prebiotic effects. However, insight into the specificity of individual GH42 enzymes with respect to substrate monosaccharide composition, glycosidic linkage and degree of polymerization is lagging. Kinetic analysis of natural and synthetic substrates resembling various milk and plant galactooligosaccharides distinguishes the three GH42 members, Bga42A, Bga42B and Bga42C, encoded by the probiotic B. longum subsp. infantis ATCC 15697 and revealed the glycosyl residue at subsite +1 and its linkage to the terminal Gal at subsite −1 to be key specificity determinants. Bga42A thus prefers the β1-3-galactosidic linkage from human milk and other β1-3- and β1-6-galactosides with glucose or Gal situated at subsite +1. In contrast, Bga42B very efficiently hydrolyses 4-galactosyllactose (Galβ1-4Galβ1-4Glc) as well as 4-galactobiose (Galβ1-4Gal) and 4-galactotriose (Galβ1-4Galβ1-4Gal). The specificity of Bga42C resembles that of Bga42B, but the activity was one order of magnitude lower. Based on enzyme kinetics, gene organization and phylogenetic analyses, Bga42C is proposed to act in the metabolism of arabinogalactan-derived oligosaccharides. The distinct kinetic signatures of the three GH42 enzymes correlate to unique sequence motifs denoting specific clades in a GH42 phylogenetic tree providing novel insight into GH42 subspecificities. Overall, the data illustrate the metabolic adaptation of bifidobacteria to the β-galactoside-rich gut niche and emphasize the importance and diversity of β-galactoside metabolism in probiotic bifidobacteria.

General information
State: Published
Organisations: Department of Systems Biology, Enzyme and Protein Chemistry, Department of Chemistry, Organic Chemistry, Center for Nanomedicine and Theranostics, Ishikawa Prefectural University, National Agriculture and Food Research Organization, Obihiro University of Agriculture and Veterinary Medicine
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Web of Science (2018): Indexed yes
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Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 1.33 SNIP 0.845 CiteScore 2.79
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.638 SNIP 1.142 CiteScore 3.4
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.535 SNIP 0.954 CiteScore 3.04
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.655 SNIP 1.275 CiteScore 3.76
ISI indexed (2013): ISI indexed yes
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Scopus rating (2012): SJR 1.711 SNIP 1.137 CiteScore 3.41
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.573 SNIP 1.199 CiteScore 3.61
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Distribution of gas hydrate inhibitor monoethylene glycol in condensate and water systems: Experimental measurement and thermodynamic modeling using the cubic-plus-association equation of state

The deepwater energy sector represents one of the major growth areas of the oil and gas industry today. To meet the challenges of hydrate formation, corrosion, scaling, and foaming, the oil and gas industry uses many chemicals and their use has increased significantly over the years. To inhibit gas hydrate formation in subsea pipelines, monoethylene glycol (MEG) and methanol are injected in large amounts. It is important to know the distribution of these chemicals in oil and water systems for economical operation of a production facility and environmental perspective. In this work, we present new data for liquid-liquid equilibrium of North Sea condensate + MEG and North Sea condensate + MEG + water systems for temperatures from 303.15 to 323.15 K and atmospheric pressure. These data are successfully modeled using the cubic-plus-association equation of state. © 2014 American Chemical Society.
Dynamics study of green AuNP formation and their basis for Au-Pt core-shell nanostructure synthesis

The SAMENS method (saccharide-based approach to metallic nanostructure synthesis) is a synthesis platform for metallic nanostructures. The method has been developed since 2008 and can produce nanostructures of various sizes, shapes and compositions. Recently, a new methodology for studying the details of nanoparticle formation has been developed employing readily available electrochemical and optical techniques. The aim is to understand which parameters control the growth and shape and at which stages of the synthesis. The gold nanoparticles (AuNPs) studied are further used as seeds for size controlled AuNPs and Au-Pt core-shell NPs with an atomically thin Pt shell.

General information

State: Published
Organisations: Department of Chemistry, NanoChemistry
Authors: Engelbrekt, C. (Intern), Seselj, N. (Intern), Ulstrup, J. (Intern), Zhang, J. (Intern)
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Effect of Fe doping on low temperature deNOx activity of high-performance vanadia-anatase nanoparticles
VFe/TiO2 catalysts have been prepared using a sol-gel based method. Fe was introduced using 3 different methods. The resulting substances were characterized with N2-physisorption, NH3-TPD, H2-TPR, XPS and XRD. Extrudates of the VFe/TiO2 powders were prepared using sepiolite (20 wt.%) as binder. The activities of the composite materials in the selective catalytic reduction (SCR) of NO with NH3 were measured at temperatures of up to 200 °C and in the presence of 20 vol. % H2O. Presence of Fe can increase the surface area, enhance the redox properties, increase the number of surface acid sites, increase the share of surface adsorbed oxygen and does not induce the formation of crystalline V2O5. However, the measurements performed here show that Fe doping does not cause activity enhancement of the V/TiO2.

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Department of Chemical and Biochemical Engineering, CHEC Research Centre
Authors: Schill, L. (Intern), Putluru, S. S. R. (Intern), Jensen, A. D. (Intern), Fehrmann, R. (Intern)
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Journal: Catalysis Communications
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BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.33 SJR 0.91 SNIP 0.95
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.998 SNIP 1.129 CiteScore 3.55
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.162 SNIP 1.321 CiteScore 3.81
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.206 SNIP 1.283 CiteScore 3.6
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.165 SNIP 1.438 CiteScore 3.2
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.253 SNIP 1.502 CiteScore 3.51
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.319 SNIP 1.254
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.16 SNIP 1.26
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.104 SNIP 1.33
Efficient epoxidation of propene using molecular catalysts

The epoxidation of propene is performed in homogeneous phase using various molecular catalysts and H2O2 or tert-butyl hydroperoxide as oxidants. A comparison between some molybdenum catalysts and methyltrioxorhenium (MTO) shows that the well known Re catalyst is the best among the examined catalysts.

General information
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Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Technische Universität München
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Main Research Area: Technical/natural sciences

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Journal: Catalysis Science & Technology
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BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
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Scopus rating (2016): CiteScore 5.64 SJR 1.795 SNIP 1.288
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.838 SNIP 1.319 CiteScore 5.46
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.897 SNIP 1.485 CiteScore 5.44
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.776 SNIP 1.343 CiteScore 4.89
ISI indexed (2013): ISI indexed yes
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Electroactive Functionalization of Graphene as Nanohybrid Materials for Redox Sensing and Energy Storage

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Organisations: Department of Chemistry, NanoChemistry
Authors: Chi, Q. (Intern), Zhu, N. (Intern), Gan, S. (Intern), Ulstrup, J. (Intern), Zhang, P. (Intern)
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Enzyme catalysed production of sialylated human milk oligosaccharides and galactooligosaccharides by Trypanosoma cruzi trans-sialidase

A Trypanosoma cruzi trans-sialidase (E.C. 3.2.1.18) was cloned into Pichia pastoris and expressed. The pH and temperature optimum of the enzyme was determined as pH 5.7 and 30°C. Using casein glycomacropeptide (CGMP) and lactose as sialyl-donor and acceptor respectively, the optimal donor/acceptor ratio for the trans-sialidase catalysed 3'-sialyllactose production was found to be 1:4. Quantitative amounts of 3'-sialyllactose were produced from CGMP and lactose at a yield of 40mg/g CGMP. The 3'-sialyllactose obtained exerted a stimulatory effect on selected probiotic strains, including different Bifidobacterium strains in single culture fermentations. The trans-sialidase also catalysed the transfer of sialic acid from CGMP to galacto-oligosaccharides (GOS) and to the human milk oligosaccharide (HMO) backbone lacto-N-tetraose (LNT) to produce 3'-sialyl-GOS, including doubly sialylated GOS products, and 3'-sialyl-LNT, respectively. This work thus provides proof of the concept of producing 3'-sialyllactose and potentially other sialylated HMOs as well as sialylated GOS enzymatically by trans-sialidase activity, while at the same time providing valorisation of CGMP, a co-processing product from cheese manufacture.

General information
State: Published
Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, Organic Chemistry, Department of Chemistry, University of Southern Denmark, DuPont Nutrition and Health
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Main Research Area: Technical/natural sciences

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Scopus rating (2016): CiteScore 3.67 SJR 1.065 SNIP 1.269
Exploring the Local Elastic Properties of Bilayer Membranes Using Molecular Dynamics Simulations

Membrane mechanical elastic properties regulate a variety of cellular processes involving local membrane deformation, such as ion channel function and vesicle fusion. In this work, we used molecular dynamics simulations to estimate the local elastic properties of a membrane. For this, we calculated the energy needed to extract a DOPE lipid molecule, modified with a linker chain, from a POPC bilayer membrane using the umbrella sampling technique. Although the extraction energy entails several contributions related not only to elastic deformation but also to solvation, careful analysis of the potential of mean force (PMF) allowed us to dissect the elastic contribution. With this information, we calculated an effective linear spring constant of 44 ± 4 kJ·nm⁻²·mol⁻¹ for the DOPC membrane, in agreement with experimental estimates. The membrane deformation profile was determined independently during the stretching process in molecular detail, allowing us to fit this profile to a previously proposed continuum elastic model. Through this approach, we calculated an effective membrane spring constant of 42 kJ²·mol⁻¹, which is in good agreement with the PMF calculation. Furthermore, the solvation energy we derived from the data is shown to match the solvation energy estimated from critical micelle formation constants. This methodology can be used to determine how changes in lipid composition or the presence of membrane modifiers can affect the elastic properties of a membrane at a local level.
Extending the hydrophobic cavity of β-cyclodextrin results in more negative heat capacity changes but reduced binding affinities

The formation of inclusion complexes of hydroxypropylated β-cyclodextrins (CDs) with three bile salts are investigated to shed light on the role played by the hydroxypropyl (HP) substituents. The HP-chains are situated at the rim of the CD and may thus extend the hydrophobic cavity of the CD. Calorimetric titrations in a broad temperature range and molecular dynamics simulations confirm previous speculations that the HP-chains cause an increase in dehydrated nonpolar surface area upon formation of the complexes. This additional burial of nonpolar surface area, 12–16 Å² per HP-chain according to the MD simulations, results in more negative values of ΔC p °, which are in quantitative agreement with what is expected for hydrophobic dehydration. Although these observations support the picture of an extended hydrophobic cavity, HPβCD complexes were less stable than their unsubstituted counterparts. This indicates that increased hydrophobic contacts are not always accompanied by increased binding strength. The linear dependence of ΔC p °, ΔH° and ΔS° on the number of HP-chains give rise to isoentropic and isoenthalpic temperatures at which ΔH° and ΔS° are independent of the number of HP-chains on the host CD (but depend on the type of bile salt). Interestingly, these convergence temperatures are close to what is observed for unfolding of proteins and may be a common feature of hydrophobic dehydration.

General information
State: Published
Organisations: Department of Chemistry, Physical and Biophysical Chemistry, Roskilde University, H. Lundbeck A/S
Authors: Schönbeck, C. (Forskerdatabase), Holm, R. (Forskerdatabase), Westh, P. (Ekstern), Peters, G. H. (Intern)
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BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.34 SNIP 0.484 CiteScore 1.09
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.314 SNIP 0.57 CiteScore 1.32
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.455 SNIP 0.72 CiteScore 1.45
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.445 SNIP 0.6 CiteScore 1.37
ISI indexed (2013): ISI indexed no
Familial placement of Wightia (Lamiales)

The familial placement of Wightia has long been a problem. Here, we present a comprehensive phylogenetic inspection of Wightia based on noncoding chloroplast loci (the rps16 intron and the tmL−F region) and nuclear ribosomal internal transcribed spacer, and on chemical analysis. A total of 70 samples (including 51 genera from 13 families of Lamiales) were employed in a molecular study. Phylograms suggest that Wightia is sister to Paulownia or Phrymaceae; species tree shows Wightia and Paulownia are sister groups which clustered with Phrymaceae in an unresolved clade. Chemical evidence shows affinity of Wightia to Paulowniaceae. With the addition of morphological, palynological and ecological characters, we suppose a familial position of Wightia belonging to or close to Paulowniaceae. Brandisia (a member of Orobanchaceae) does not have a close relationship with Wightia.

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry, East China Normal University
Authors: Zhou, Q. (Ekstern), Jensen, S. R. (Intern), Liu, G. (Ekstern), Wang, S. (Ekstern), Li, H. (Ekstern)
Pages: 2009-2017
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Journal: Plant Systematics and Evolution
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BFI (2018): BFI-level 1
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Web of Science (2017): Indexed Yes
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Scopus rating (2016): CiteScore 1.39 SJR 0.595 SNIP 0.975
Femtochemistry – some reflections and perspectives

In this perspective we highlight some aspects of femtochemistry, that is, the creation, detection and control of non-stationary states in chemical dynamics. Some recent results are discussed with a view on the challenges and pending scientific questions. We discuss theoretical as well as experimental issues with the emphasis on laser control of chemical dynamics, in the weak-field and strong-field regimes.

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State: Published
Organisations: Department of Chemistry, Physical and Biophysical Chemistry
Authors: Henriksen, N. E. (Intern)
Pages: 2-8
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Journal: Chemical Physics
Volume: 442
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Ratings:
Fermi Potential across Working Solid Oxide Cells with Zirconia or Ceria Electrolytes

A solid electrolyte will always possess a finite electronic conductivity, in particular electrolytes like doped ceria that easily get reduced and become mixed ionic and electronic conductors. This given rise too high leak currents through the solid oxide cell (SOC). Especially, problems have been observed for ceria based electrolytes, but also in case of solid oxide electrolyser cells (SOEC) with yttria stabilized zirconia (YSZ) big electronic leak currents have been observed for very high overvoltages on one or both electrodes. Furthermore, it is important to realize that the potential gradient driving the O2-ions is not the Fermi potential, which is the potential of the electrons, but the Galvani potential (or inner potential) (1). The concepts of potentials describing the electrical situation of a solid electrolyte is shown i Fig. 1, and an example of the Fermi potential (π) and Galvani potential (φ) profiles are shown in Fig. 2. The Fermi potential will be affected directly by the Galvani potential, whereas the Galvani potential need not necessarily be affected by the Fermi potential because the concentration of "free" electrons may be very low. The paper gives illustrative examples at various temperatures and operation conditions. Furthermore, the situation within cells based on gadolinia doped ceria (CGO) and on YSZ electrolytes are compared. Finally, it is discussed how the Fermi potential and electron conductivity will be affected by the various parameters including operation conditions. Reference [1] T. Jacobsen and M. Mogensen, ECS Transactions, 13 (no.26), 259 (2008).
The nuclease domain of colicin E7 (NColE7) promotes the nonspecific cleavage of nucleic acids at its C-terminal HNH motif. Interestingly, the deletion of four N-terminal residues (446–449NColE75KRNK) resulted in complete loss of the enzyme activity. R447A mutation was reported to decrease the nuclease activity, but a detailed analysis of the role of the highly positive and flexible N-terminus is still missing. Here, we present the study of four mutants, with a decreased activity in the following order: NColE7>>KGNK > KGNG~GGNK > GGNG. At the same time, the folding, the metal-ion, and the DNA-binding affinity were unaffected by the mutations as revealed by linear and circular dichroism spectroscopy, isothermal calorimetric titrations, and gel mobility shift experiments. Semiempirical quantum chemical calculations and molecular dynamics simulations revealed that K446, K449, and/or the N-terminal amino group are able to approach the active centre in the absence of the other positively charged residues. The results suggested a complex role of the N-terminus in the catalytic process that could be exploited in the design of a controlled nuclease.
Flue Gas Cleaning

Flue gases from industrial sources like power, waste incineration, glass manufacturer and cement plants as well as ships meet increasingly stricter regulations regarding emission of several pollutants in particular nitrogen and sulfur oxides. These pollutants lead to formation of nitric and sulfuric acid in the atmosphere causing precipitation of acid rain resulting in death of forests and destruction of buildings and monuments in addition to human health problems. The most common state-of-the-art methods applied today industrially for cleaning of flue gases will be addressed, including wet and dry...
scrubbing for sulfur oxides (SO2) and catalytic removal of nitrogen oxides (NOx). There is however, a desire of increasing the energy produced in electrical power plants by firing CO2-neutral biomass/waste or biomass/waste in combination with fossil fuels. Thus, the EU reached agreement in March 2007 specifying that 20 % and recently in 2014 this was increased to 40 % of the energy should be produced from renewable fuels by 2020 and 2030, respectively to cut emissions of the greenhouse gas CO2. This, however, challenges not only the power plant itself due to enhanced slagging, fouling and corrosion, but also the downstream cleaning of the flue gas for nitrogen oxides (NOx) which is almost exclusively carried out using selective catalytic reduction (SCR) with ammonia (NH3) as reductant. It is now well known that the traditional industrial catalyst used for SCR of NOx by ammonia is severely deactivated by the aggressive flue gas, originating from the high content of potassium salts found in the biomass compared to fossil fuels. Also the formation of large amounts of more or less useful gypsum by the traditional lime scrubbing for sulfur oxides in the flue gas pose an increasingly new waste problem. In Centre for Catalysis and Sustainable Chemistry, DTU Chemistry we are carrying out research dedicated to solve this problem not only by traditional catalytic routes where we from a molecular understanding of the catalyst performance try to improve the composition and catalyst life-time. But the problems may also be attacked by new materials like supported ionic liquid phase (SILP) gas absorbers where the pollutants may be selectively absorbed, desorbed and finally converted to useful mineral acids of commercial grade – really a green waste-to-value approach that we persue instead of the traditional cleaning processes that use chemicals to form new wastes.

General information
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Authors: Fehrmann, R. (Intern)
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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.

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Authors: Mielby, J. J. (Intern), Abildstrøm, J. O. (Intern), Perez-Ferreras, S. (Ekstern), Rasmussen, S. B. (Intern), Kegnæs, S. (Intern)
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Web of Science (2017): Indexed Yes
Graphene controlled H- and J-stacking of perylene dyes into highly stable supramolecular nanostructures for enhanced photocurrent generation.

We report a new method for controlling H- and J-stacking in supramolecular self-assembly. Graphene nanosheets act as structure inducers to direct the self-assembly of a versatile organic dye, perylene into two distinct types of functional nanostructures, i.e. one-dimensional nanotubes via J-stacking and two-dimensional branched nanobuds through H-stacking. Graphene integrated supramolecular nanocomposites are highly stable and show significant enhancement of photocurrent generation in these two configurations of photosensing devices, i.e. solid-state optoelectronic constructs and liquid-junction solar cells.
Graphene Nanofilms Functionalized with Electroactive Nanoparticles and Enzyme for Electrocatalytic Sensing

General information
State: Published
Organisations: Department of Chemistry, NanoChemistry
Authors: Zhu, N. (Intern), Han, S. (Intern), Dey, R. S. (Intern), Ulstrup, J. (Intern), Chi, Q. (Intern)
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Green synthesis and structural control of metal and mineral nanostructures
Nanomaterials are widely used in modern technology, especially as catalysts in energy technology. Nanocatalysts are often prepared from expensive elements that constitute a large part of the total device cost. A critical component in the successful implementation of sustainable energy technology is efficiency which in large part comes down to the efficiency
of the catalyst. Global issues arising from the use and reliance on fossil fuels urges the transition to sustainable alternatives and the development of new highly efficient nanomaterials. The efficiency depends on structure so controlling size, shape and composition at the atomic level is essential. To this adds low cost if massive use is anticipated. In this work, nanostructures of gold, platinum/gold, platinum/palladium, clinoatacamite (Cu₂(OH)₃Cl), cupric oxide and gold/titanium dioxide were synthesized and broadly characterized, their formation mechanisms studied, and their application as catalysts in relevant systems tested. Solution synthesis of nanomaterials offers large-scale, mild production but control of size, shape and composition is often challenging. This may be improved by expanding the understanding of the complex processes of nanoparticle formation which, however, entails the development of new methods. Two approaches to the advancement of solution synthesis of gold nanomaterials for energy technology were exploited, namely the development of techniques to study nanoparticle formation and the synthesis of active, composite nanomaterials. In the first approach, time-resolved chronopotentiometry, pH, conductivity and turbidity, and ultraviolet-visible light spectroscopy were employed to follow the green synthesis of gold nanoparticles. Several distinct phases were observed with all techniques providing a broad picture of the complex processes. Strong indications of sequential reduction were found and details about ligands and surface immobilized molecules disclosed. This platform is a widely available alternative to traditionally used synchrotron techniques. In the second approach, systematic efforts toward size and shape control of gold nanostructures provided controlled synthesis of not only spherical gold nanoparticles of 8-80 nm but also graphene oxide templated preparation of flat, ring-shaped gold nanostructures up to 1 μm in diameter mainly exposing (111) facets. Increased efficiency of new platinum nanocatalysts was attempted by two parallel strategies. One entailed avoiding inactive bulk platinum using a gold core and leaving only vi an atomically thin platinum shell. The specific catalytic activity of this nanocomposite will be studied in the future. The other strategy was to alloy platinum with a cheaper element, i.e. palladium, while retaining high activity. Supported PdPt alloy nanoparticles were successfully prepared and showed promising performance as catalysts in direct methanol and formic acid fuel cells. Catalysts made from earth-abundant elements may provide other low-cost alternatives to traditional, scarce and expensive catalysts. This may be achieved through niche applications and nanoscale engineering. Copper mineral nanoparticles were prepared and studied for this purpose. A buffered synthesis offering the preparation of phase-pure clinoatacamite Cu₂(OH)₃Cl and tenorite CuO by controlling pH was developed. Detailed crystallographic characterization was obtained by combining X-ray diffraction and infrared spectroscopy. The synthesis of CuO was further optimized and the flat, rod-shaped nanostructures applied as heterogeneous catalysts for oxidative dehydrogenation reactions. High activity and good reusability was found and the potential of this noble metal-free system will be explored further. Solar energy is appealing as a plentiful and free energy source. A plasmonic photoelectrocatalytic system was prepared to utilize visible light by incorporating gold nanoparticles in titania. The composite material showed improved optical properties compared to pure titanium dioxide and preliminary catalytic tests were promising.

**General information**

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Authors: Engelbrekt, C. (Intern), Zhang, J. (Intern), Ulstrup, J. (Intern)

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Christian_Engelbrekt.pdf

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Guanidino groups greatly enhance the action of antimicrobial peptidomimetics against bacterial cytoplasmic membranes. Antimicrobial peptides or their synthetic mimics are a promising class of potential new antibiotics. Herein we assess the effect of the type of cationic side chain (i.e., guanidino vs. amino groups) on the membrane perturbing mechanism of antimicrobial α-peptide-β-peptoid chimeras. Langmuir monolayers composed of 1,2-dipalmitoyl-sn-glycero-3-phosphatidylglycerol (DPPG) were used to model cytoplasmic membranes of both Gram-positive and Gram-negative bacteria, while lipopolysaccharide Kdo2-lipid A monolayers were mimicking the outer membrane of Gram-negative species. We report the results of the measurements using an array of techniques, including high-resolution synchrotron surface X-ray scattering, epifluorescence microscopy, and in vitro antimicrobial activity to study the molecular mechanisms of peptidomimetic interaction with bacterial membranes. We found guanidino group-containing chimeras to exhibit greater disruptive activity on DPPG monolayers than the amino group-containing analogues. However, this effect was not observed for lipopolysaccharide monolayers where the difference was negligible. Furthermore, the addition of the nitrobenzoxadiazole fluorophore did not reduce the insertion activity of these antimicrobials into both model membrane systems examined, which may be useful for future cellular localization studies.

**General information**

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Hexamethylcyclopentadiene: time-resolved photoelectron spectroscopy and ab initio multiple spawning simulations

Progress in our understanding of ultrafast light-induced processes in molecules is best achieved through a close combination of experimental and theoretical approaches. Direct comparison is obtained if theory is able to directly reproduce experimental observables. Here, we present a joint approach comparing time-resolved photoelectron spectroscopy (TRPES) with ab initio multiple spawning (AIMS) simulations on the MS-MR-CASPT2 level of theory. We disentangle the relationship between two phenomena that dominate the immediate molecular response upon light absorption: a spectrally dependent delay of the photoelectron signal and an induction time prior to excited state depopulation in dynamics simulations. As a benchmark molecule, we have chosen hexamethylcyclopentadiene, which shows an unprecedentedly large spectral delay of (310 ± 20) fs in TRPES experiments. For the dynamics simulations, methyl groups were replaced by “hydrogen atoms” having mass 15 and TRPES spectra were calculated. These showed an induction time of (108 ± 10) fs which could directly be assigned to progress along a torsional mode leading to the intersection seam with the molecular ground state. In a stepladder-type approach, the close connection between the two phenomena could be elucidated, allowing for a comparison with other polyenes and supporting the general validity of this finding for their excited state dynamics. Thus, the combination of TRPES and AIMS proves to be a powerful tool for a thorough understanding of ultrafast excited state dynamics in polyenes.
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.
High-resolution infrared spectroscopy of CH281BrF near 8 μm: rovibrational analysis of the ν3 and ν8 fundamentals and resonances with the dark states 2ν5 and ν6 + ν9

The infrared spectrum of isotopically enriched CH2 81BrF was investigated in the ν3 and ν8 region between 1150 and 1370 cm−1 at a resolution of 0.003 cm−1. The ν3 vibration of symmetry species A gives rise to an a-/b-hybrid band with a-type predominance, while the ν8 mode of A symmetry produces c-type absorption. Due to the proximity of the band origins to those of closely lying overtones and combination bands, the ν3 = 1 and ν8 = 1 levels were found perturbed through Coriolis resonance by the ν5 = 2 (A) and ν6 = ν9 = 1 (A) states, respectively. The spectral analysis resulted in the identification of 3132 transitions (J ≤ 98 and Ka ≤ 14) for the ν3 and 2958 transitions (J ≤ 68 and Ka ≤ 19) for the ν8 bands. The assigned data were fitted using the Watson’s A-reduction Hamiltonian in the Ir representation and the perturbation operators. Although no transitions belonging to the perturbers were observed, the band origins and excited state parameters for fundamentals and ‘dark states’ together with coupling terms for the ν3/2ν5 and ν8/ν6 + ν9 dyads were determined.

General information
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Organisations: Department of Chemistry, Università Ca’ Foscari Venezia
Authors: Stroppa, P. (Ekstern), Tasinato, N. (Ekstern), Baldacci, A. (Ekstern), Pietropolli Charmeta, A. (Ekstern), Giorgianni, S. (Ekstern), Larsen, R. W. (Intern)
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Scopus rating (2016): CiteScore 1.65 SJR 0.833 SNIP 0.729
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.761 SNIP 0.85 CiteScore 1.68
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.697 SNIP 0.667 CiteScore 1.48
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.678 SNIP 0.715 CiteScore 1.58
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.801 SNIP 0.738 CiteScore 1.62
ISI indexed (2012): ISI indexed yes
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BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.824 SNIP 0.829 CiteScore 1.67
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.786 SNIP 0.722
BFI (2009): BFI-level 1
Hydroformylation of olefins and reductive carbonylation of aryl halides with syngas formed ex situ from dehydrogenative decarbonylation of hexane-1,6-diol.

A variety of primary alcohols have been investigated as convenient substrates for the ex situ delivery of carbon monoxide and molecular hydrogen in a two-chamber reactor. The gaseous mixture is liberated in one chamber by an iridium-catalysed dehydrogenative decarbonylation of the alcohol and then consumed in the other chamber in either a rhodium-catalysed hydroformylation of olefins or a palladium-catalysed reductive carbonylation of aryl halides. Hexane-1,6-diol was found to be the optimum alcohol for both reactions where moderate to excellent yields were obtained of the product aldehydes. A relatively low pressure of 1.5-2.4 bar was measured in the closed system during the two transformations.
Fe/TiO2 based catalysts were prepared by incipient wetness impregnation and deposition–precipitation (DP). The catalysts were characterized by activity measurements, N2 physisorption, X-ray powder diffraction, electron paramagnetic resonance spectroscopy, energy dispersive X-ray spectroscopy, H2-temperature programmed reduction and NH3-temperature programmed desorption. The 3 wt% Fe–10 wt% WO3/TiO2 (3Fe–10WTi-DP) catalyst prepared by DP using ammonium carbamate as a precipitating agent was found to be the most active and hydrothermally stable with 11 vol% H2O in air at 650 °C for 3 h. The hydrothermal stability of the catalyst can be attributed to the retained crystal structure, and mild change in acidic and redox properties of the catalyst. Furthermore, hydrothermal stability of the 3Fe–10WTi-DP catalyst is competitive with that of 3Fe–ZSM-5 and much better than 3V2O5–10WO3–TiO2 catalysts. Relative SCR activity of catalysts at 450 °C.
Impact of soil amendments and the plant rhizosphere on PAH behaviour in soil

Carbonaceous amendments reduce PAH dissolved concentrations ($C_{\text{free}}$), limiting their uptake and toxicity. A soil contaminated with PAHs was mixed with activated carbon (AC), charcoal or compost and planted with radish (Raphanus sativus L.), and $C_{\text{free}}$ chemical activities and diffusive uptake of the PAHs measured over 2 months. For AC, $C_{\text{free}}$ and diffusive uptake were decreased by up to 94% compared to the unamended soil within one week. In addition, the sum chemical activity of the PAHs remained below the threshold for baseline toxicity. In contrast, charcoal and compost only led to modest reductions in $C_{\text{free}}$ and diffusive uptake, with sum chemical activities that could potentially result in baseline toxicity being observed. Furthermore, both $C_{\text{free}}$ and diffusive uptake were lower in the planted compared to unplanted soils. Therefore, only AC successfully reduced PAH acute toxicity in the soil, but plant-promoted microbial degradation may also play an important role in PAH attenuation.

General information
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Organisations: Department of Chemistry, CERE – Center for Energy Resources Engineering, Department of Environmental Engineering, Environmental Chemistry, Universität des Saarlandes, Aarhus University
Authors: Marchal, G. (Intern), Smith, K. E. (Ekstern), Mayer, P. (Intern), Wollesen de Jonge, L. (Ekstern), Karlson, U. G. (Ekstern)
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Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 5.27 SJR 1.786 SNIP 1.729
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 2.002 SNIP 1.73 CiteScore 4.72
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.986 SNIP 2.03 CiteScore 4.57
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.973 SNIP 1.944 CiteScore 4.35
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 2.063 SNIP 1.744 CiteScore 4.03
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 2.043 SNIP 1.741 CiteScore 3.87
ISI indexed (2011): ISI indexed yes
Biocatalytic trans-sialylation is relevant for the design of biomimetic oligosaccharides such as human milk oligosaccharides. t-Butanol and ionic liquids, EAN (ethylammonium nitrate), [MMIm][MeSO4] (1,3-dimethylimidazolium methyl sulfate), and [C2OHMIm][PF6] (1-(2-hydroxyethyl)-3-methylimidazolium hexafluorophosphate), were examined as co-solvents for the improvement of the synthesis versus hydrolysis ratio in the trans-sialylation of lactose, catalysed by an engineered sialidase from Trypanosoma rangeli. The use of 25 % (v/v) t-butanol as co-solvent significantly increased 3'-sialyllactose production by 40 % from 1.04 ± 0.09 to 1.47 ± 0.01 mM. The synthesis versus hydrolysis ratio increased correspondingly by 1.2-times. 1-2.5 % (v/v) EAN or [C2OHMIm][PF6] improved the synthesis versus hydrolysis ratio up to 2.5-times but simultaneously decreased the 3'-sialyllactose yield, probably due to enzyme inactivation caused by the ionic liquid. [MMIm][MeSO4] had a detrimental effect on the trans-sialylation yield and on the ratio between synthesis and hydrolysis.

**General information**

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Organisations: Department of Chemical and Biochemical Engineering, Center for BioProcess Engineering, Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Technical University of Denmark
Authors: Zeuner, B. (Intern), Riisager, A. (Intern), Mikkelsen, J. D. (Intern), Meyer, A. S. (Intern)
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Scopus rating (2016): CiteScore 1.89 SJR 0.61 SNIP 0.721
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.591 SNIP 0.673 CiteScore 1.66
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.627 SNIP 0.809 CiteScore 1.75
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.713 SNIP 0.941 CiteScore 2.03
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.758 SNIP 0.949 CiteScore 2.03
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.722 SNIP 0.912 CiteScore 1.97
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.698 SNIP 0.894
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.707 SNIP 0.816
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.628 SNIP 0.778
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.533 SNIP 0.725
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 0.543 SNIP 0.718
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.462 SNIP 0.68
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.455 SNIP 0.602
Scopus rating (2003): SJR 0.44 SNIP 0.635
Scopus rating (2002): SJR 0.477 SNIP 0.658
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.528 SNIP 0.85
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HASH(0x4772848), t-Butanol, Casein glycomacropeptide (CGMP), Co-solvent, Ionic liquids, 3’Sialyllactose, trans-Sialidase, Trypanosoma rangeli

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10.1007/s10529-014-1488-3
Incorporation of tin affects crystallization, morphology, and crystal composition of Sn-Beta.

The crystallization of Sn-Beta in fluoride medium is greatly influenced by the amount and type of tin source present in the synthesis gel. By varying the amount of tin in the form of tin(IV) chloride pentahydrate, the time required for crystallization was studied. It was found that tin not only drastically affects the time required for crystallization, but also that the presence of tin changes the morphology of the formed Sn-Beta crystals. For low amounts of tin (Si/Sn ¼ 400), crystallization occurs within four days and the Sn-Beta crystals are capped bipyramidal in shape, whereas for high amounts of tin (Si/Sn ¼ 100), it takes about sixty days to reach full crystallinity and the resulting crystals are highly truncated, almost plate-like in shape. Using SEM-WDS to investigate the tin distribution along transverse sections of the Sn-Beta crystals, a gradient distribution of tin was found in all cases. It was observed that the tin density in the outer parts of the Sn-Beta crystals is roughly twice as high as in the tin depleted core of the crystals. Sn-Beta was found to obtain its maximum catalytic activity for the conversion of dihydroxyacetone to methyl lactate close to the minimum time required for obtaining full crystallinity. At excessive crystallization times, the catalytic activity decreased, presumably due to Ostwald ripening.

In-situ annotation of carbohydrate diversity, abundance, and degradability in highly complex mixtures using NMR spectroscopy.

Many functions of carbohydrates depend on the detection of short structural motifs, approximately up to hexasaccharide length, by receptors or catalysts. This study investigates the usefulness of state-of-the-art $^1$H-$^{13}$C nuclear-magnetic-resonance (NMR) spectroscopy for characterizing the diversity, abundance, and degradability of such short structural motifs in plant-derived carbohydrates. Assignments of carbohydrate signals for $^1$H-$^{13}$C NMR spectra of beer, wine, and
fruit juice yield up to >130 assignments in situ, i.e. in individual samples without separation or derivatization. More than 500 structural motifs can be resolved over a concentration range of $\sim 10^3$ in experiments of a few hours duration. The diversity of carbohydrate units increases according to power laws at lower concentrations for both cereal and fruit-derived samples. Simple graphs resolve the smaller overall contribution of more diverse but less abundant motifs to carbohydrate biomass. Susceptibility to enzymatic degradation is probed simultaneously for hundreds of structural motifs to reduce uncertainties in the identification of motifs and to probe enzyme specificity with assigned motifs. Several properties of fundamental biotechnological importance can thus be assessed in situ by heteronuclear NMR methods.

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Organisations: Department of Chemistry, Organic Chemistry  
Authors: Meier, S. (Intern)  
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Scopus rating (2016): CiteScore 3.03 SJR 0.943 SNIP 1.039  
Web of Science (2016): Indexed yes  
BFI (2015): BFI-level 1  
Scopus rating (2015): SJR 1.064 SNIP 1.083 CiteScore 3.07  
Web of Science (2015): Indexed yes  
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Scopus rating (2014): SJR 1.126 SNIP 1.222 CiteScore 3.26  
Web of Science (2014): Indexed yes  
BFI (2013): BFI-level 1  
Scopus rating (2013): SJR 1.229 SNIP 1.282 CiteScore 3.55  
ISI indexed (2013): ISI indexed yes  
Web of Science (2013): Indexed yes  
BFI (2012): BFI-level 1  
Scopus rating (2012): SJR 1.347 SNIP 1.282 CiteScore 3.51  
ISI indexed (2012): ISI indexed yes  
Web of Science (2012): Indexed yes  
BFI (2011): BFI-level 1  
Scopus rating (2011): SJR 1.363 SNIP 1.275 CiteScore 3.47  
ISI indexed (2011): ISI indexed yes  
Web of Science (2011): Indexed yes  
BFI (2010): BFI-level 1  
Scopus rating (2010): SJR 1.354 SNIP 1.236  
Web of Science (2010): Indexed yes  
BFI (2009): BFI-level 1  
Scopus rating (2009): SJR 1.272 SNIP 1.237  
Web of Science (2009): Indexed yes  
BFI (2008): BFI-level 1  
Scopus rating (2008): SJR 1.144 SNIP 1.076  
Web of Science (2008): Indexed yes  
Scopus rating (2007): SJR 1.08 SNIP 1.096
In situ surface reduction of a NiO-YSZ-Al2O3 composite using scanning probe microscopy

In situ surface reductions of NiO-YSZ-Al2O3 composites into Ni-YSZ-Al2O3 cermets were carried out at 312–525 °C in a controlled atmosphere high-temperature scanning probe microscope (CAHT-SPM) in dry and humidified 9 % H2 in N2. The reduction of NiO was followed by contact mode scanning of topography and conductance. A reproducible sequence of events was observed which included a conductance decrease upon hydrogen introduction and a reappearance of conductance after some time. It was found that this incubation time from introduction of hydrogen and until conducting Ni appeared was temperature dependent and followed the Arrhenius equation. For samples reduced in dry hydrogen, the Arrhenius plot showed two regions with different activation energies. Scanning electron microscopy confirmed a difference in microstructure between these temperature regimes. A strong retarding effect of steam (H2O) on the nucleation time of Ni particles was observed.

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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.26 SJR 0.662 SNIP 0.721
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.652 SNIP 0.679 CiteScore 2.18
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.834 SNIP 1.009 CiteScore 2.59
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.735 SNIP 0.926 CiteScore 2.25
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Supercapacitors are a kind of efficient and safe energy storage and conversion devices. The development of new-generation supercapacitors that can be used in portable electronic devices and in next-generation vehicles is increasingly demanded. This crucially depends on the discovery of more efficient and cost-effective novel materials. Because of their ultrahigh specific surface areas and excellent conductivity, three-dimensional (3D) graphene materials hold great promises for supercapacitors. However, the assembly of graphene building blocks into the supercapacitor electrodes with low intrinsic resistance and high ion conductance is still a challenging issue. In this work, we have undertaken the challenge and used electrochemically generated copper foams (CuF) as an effective template to directly integrate reduced graphene oxide (rGO) 3D networks. This has led to the construction of all-in-one supercapacitor electrodes (3DrGO@CuF) [1]. The overall procedure in clude s two step s: self-assembly of graphene oxide (GO) on Cu F and electrochemical reduction of GO into rGO. The resulting electrodes are capable of delivering a specific capacitance as high as 623 F g⁻¹ with high cycling stability. Thus, we have shown that high specific capacitance can be achieved with 3D graphene nanostructures without any external pseudo-capacitive species doped [2, 3]. The new method is also cost-effective and environmentally friendly.

General information
State: Published
Organisations: Department of Chemistry, NanoChemistry, University of Copenhagen
Authors: Dey, R. S. (Ekstern), Chi, Q. (Intern)
Publication date: 2014
Event: Abstract from 5th Symposium on Carbon Nanomaterials, Copenhagen, Denmark.
Main Research Area: Technical/natural sciences
Interaction of neurotransmitters with a phospholipid bilayer

We have performed a series of molecular dynamics simulations to study the interactions between the neurotransmitters (NTs) γ-aminobutyrate (GABA), glycine (GLY), acetylcholine (ACH) and glutamate (GLU) as well as the amidated/acetylated γ-aminobutyrate (GABA\text{\textsubscript{neu}}) and the osmolyte molecule glycerol (GOL) with a dipalmitoylphosphatidylcholine (DPPC) bilayer. In agreement with previously published experimental data, we found the lowest membrane affinity for the charged molecules and a moderate affinity for zwitterionic and polar molecules. The affinity can be ranked as follows: ACH–GLU << GABA < GLY << GABA\text{\textsubscript{neu}} << GOL. The latter three penetrated the bilayer at most with the deepest location being close to the glycerol backbone of the phospholipids. Even at that position, these solutes were noticeably hydrated and carried ~30–80% of the bulk water along. The mobility of hydration water at the solute is also affected by the penetration into the bilayer. Two time scales of exchanging water molecules could be determined. In the bulk phase, the hydration layer contains ~20% slow exchanging water molecules which increases 2–3 times as the solutes entered the bilayer. Our results indicate that there is no intermediate exchange of slow moving water molecules from the solutes to the lipid atoms and vice versa. Instead, the exchange relies on the reservoir of unbounded (“free”) water molecules in the interfacial bilayer region. Results from the equilibrium simulations are in good agreement with the results from umbrella sampling simulations, which were conducted for the four naturally occurring NTs. Free energy profiles for ACH and GLU show a minimum of ~2–3 kJ/mol close to the bilayer interface, while for GABA and GLY, a minimum of respectively ~2 kJ/mol and ~5 kJ/mol is observed when these NTs are located in the vicinity of the lipid glycerol backbone. The most important interaction of NTs with the bilayer is the charged amino group of NTs with the lipid phosphate group.

General information

State: Published
Organisations: Department of Chemistry, Physical and Biophysical Chemistry, Technical University of Denmark, Roskilde University
Number of pages: 11
Pages: 7-17
Publication date: 2014
Main Research Area: Technical/natural sciences

Publication information
Journal: Chemistry and Physics of Lipids
Volume: 184
ISSN (Print): 0009-3084
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.976 SNIP 0.862 CiteScore 2.78
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.957 SNIP 0.957 CiteScore 2.75
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.885 SNIP 1.039 CiteScore 2.62
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.82 SNIP 1.055 CiteScore 2.66
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.803 SNIP 0.974 CiteScore 2.41
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Few reactions can compete with the Diels-Alder (DA) [4+2] cycloaddition for the rapid and efficient generation of molecular complexity. The DA reaction is atom-economic and stereospecific, as well as diastereo- and regioselective. The intramolecular version (IMDA) of the DA cycloaddition and its transannular (TADA) counterpart are the subjects of this chapter, which covers major advances made since the first edition of Comprehensive Organic Synthesis. The chapter deals first with type 1 and type 2 IMDA cycloaddition, with a discussion on the effect of the nature of the tether linking diene and dienophile, methods for acceleration of IMDA reactions (such as use of high pressure) and catalysis (using oxophilic or carbophilic metal complexes, Brønsted acids, and enzymes). The use of furans as diene components (IMDAF), intramolecular hetero-DA (IMHDA) and IMDA reactions with inverse electron demand are also covered. Applications of IMDA to asymmetric synthesis (from substrate control through to enantioselective catalysis, including organocatalysis) are presented, along with tandem sequences involving IMDA cycloaddition. A theme pervading the whole chapter is the use of IMDA reactions for the total synthesis of complex natural products, including syntheses designed on the basis of biosynthetic proposals. The chapter concludes with an overview of the TADA cycloaddition, again with emphasis on recent total syntheses. © 2014 Elsevier Ltd. All rights reserved.
Ionic liquids as recyclable and separable reaction media in Rh-catalyzed decarbonylation of aromatic and aliphatic aldehydes

Ionic liquids (ILs) have been applied as recyclable reaction media in the decarbonylation of aldehydes in the presence of a rhodium-phosphine complex catalyst. The performance of several new catalytic systems based on imidazolium-based ILs and [Rh(dppp)2]Cl (dppp: 1,3-diphenylphosphinopropane) were excellent in the decarbonylation of both aromatic and aliphatic aldehydes providing >99 yield of benzenes and alkanes, respectively. The catalytic performance depended, however, strongly on the employed IL and its thermal stability. In addition, the ILs afforded good catalyst immobilization as well as a biphasic system with the product allowing recovery and reuse of the employed catalyst.

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Authors: Malcho, P. (Intern), Garcia-Suarez, E. J. (Intern), Riisager, A. (Intern)
Pages: 58151-58155
Publication date: 2014
Main Research Area: Technical/natural sciences

Publication information
Journal: RSC Advances
Volume: 4
Issue number: 102
ISSN (Print): 2046-2069
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.06 SJR 0.875 SNIP 0.743
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.959 SNIP 0.837 CiteScore 3.42
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.114 SNIP 0.965 CiteScore 3.87
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.117 SNIP 0.903 CiteScore 3.74
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Scopus rating (2012): SJR 0.863 SNIP 0.603 CiteScore 2.4
ISI indexed (2012): ISI indexed no
Web of Science (2012): Indexed yes
Original language: English
Aldehydes, Aromatic compounds, Catalysts, Phosphorus compounds, Rhodium, Rhodium compounds, Aliphatic aldehydes, Biphasic systems, Catalyst immobilization, Catalytic performance, Decarbonylations, Imidazolium-based, Ionic liquid (ils), Phosphine complex, Ionic liquids
DOIs:
10.1039/c4ra07103d
Source: FindIt
Isolation, Structural Analyses and Biological Activity Assays against Chronic Lymphocytic Leukemia of Two Novel Cytochalasins - Sclerotionigrin A and B

Two new cytochalasins, sclerotionigrin A (1) and B (2) were isolated together with the known proxiphomin (3) from the filamentous fungus Aspergillus sclerotioniger. The structures and relative stereochemistry of 1 and 2 were determined based on comparison with 3, and from extensive 1D and 2D NMR spectroscopic analysis, supported by high resolution mass spectrometry (HRMS). Compounds 2 and 3 displayed cytotoxic activity towards chronic lymphocytic leukemia cells in vitro, with 3 being the most active.

General information
State: Published
Organisations: Department of Systems Biology, Natural Product Chemistry, Department of Chemistry, Organic Chemistry, German Cancer Research Center (DKFZ)
Number of pages: 12
Pages: 9786-9797
Publication date: 2014
Main Research Area: Technical/natural sciences

Publication information
Journal: Molecules
Volume: 19
Issue number: 7
ISSN (Print): 1420-3049
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.09 SJR 0.809 SNIP 1.231
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.562 SNIP 1.168 CiteScore 2.65
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.725 SNIP 1.31 CiteScore 2.62
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.707 SNIP 1.283 CiteScore 2.61
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.791 SNIP 1.365 CiteScore 2.87
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.723 SNIP 1.138 CiteScore 2.54
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.561 SNIP 1.14
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.524 SNIP 1.016
Isomerisation of C4-C6 aldoses with zeolites
The present invention relates to isomerization of C4-C6 aldoses to their corresponding C4-C6 ketoses. In particular, the invention concerns isomerization of C4-C6 aldoses over solid zeolite catalysts free of any metals other than aluminum, in the presence of suitable solvent(s) at suitable elevated temperatures. C6 and C5 aldose sugars such as glucose and xylose, which are available in large amounts from biomass precursors, are isomerized to fructose and xylulose respectively, in a one or two-step process over inexpensive commercially available zeolite catalysts, containing aluminum as the only metal in the catalyst. The ketoses obtained are used as sweeteners in the food and/or brewery industry, or treated to obtain downstream platform chemicals such as lactic acid, HMF, levulinic acid, furfural, MMHB, and the like.

Laser-pulse-shape control of photofragmentation in the weak-field limit
We demonstrate theoretically that laser-induced coherent quantum interference control of asymptotic states of dissociating molecules is possible even in the (one-photon) weak-field limit starting from a single vibrational eigenstate. Thus, phase dependence in the interaction with a fixed energy phase-modulated pulse can persist for some time after the pulse is over. This is illustrated for the nonadiabatic process: \( I + Br^* \rightarrow IBr + I + Br \), where the relative yield of excited Br* can be changed by pure phase modulation. It is shown that the phase is able to influence wave-packet spreading in the continuum as well as the average internuclear distance in each channel. © 2014 American Physical Society.
Letter to the Editor regarding "Pitfalls in quality assurance".: A personal view on quality assurance

General information
State: Published
Organisations: Department of Chemistry, Analytical Chemistry
Authors: Andersen, J. E. T. (Intern)
Pages: 6081-6082
Publication date: 2014
Main Research Area: Technical/natural sciences

Publication information
Journal: Analytical and Bioanalytical Chemistry
Volume: 406
Issue number: 25
ISSN (Print): 1618-2642
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.03 SJR 0.943 SNIP 1.039
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.064 SNIP 1.083 CiteScore 3.07
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.126 SNIP 1.222 CiteScore 3.26
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.229 SNIP 1.282 CiteScore 3.55
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.347 SNIP 1.282 CiteScore 3.51
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.363 SNIP 1.275 CiteScore 3.47
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.354 SNIP 1.236
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.272 SNIP 1.237
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
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

Relations
Activities:
Summer School on Catalysis of Biomass
Publication: Research › Poster – Annual report year: 2014

Linking fungal secondary metabolites and pathways to their genes in Aspergillus
Filamentous fungi are producers of small bioactive molecules termed secondary metabolites (SMs), which display a wide range of functional and structural diversity. The compounds have several important activities including antifungal, antibacterial, anticancer, antiparasitic, antinsectan and immunosuppressive activities. The rapid increase in genomes sequences of filamentous fungi has revealed that the biosynthetic potential is enormous, due to the presence of huge numbers of biosynthetic gene clusters. Thus, there is an enormous potential of previously undiscovered SMs waiting to be exploited, which can potentially be used as pharmaceuticals. The work has focused on filamentous fungi from the important genus Aspergillus. It contains species that are both food and feed contaminants, some that are used for industrial applications for production of small compounds and enzymes, as well as model organisms for genetic studies and human opportunistic pathogens. The aim of this PhD study has been divided into two major topics:
1) Discovery and characterization of novel SMs from filamentous fungi
2) Linking genes to SMs and elucidation of biosynthetic pathways
The first part of this study, the discovery of novel SMs, has resulted in characterization of 22 novel SMs from selected Aspergilli. Two different approaches were undertaken: Dereplication based discovery and discovery by induction of sclerotium formation. The outcome included characterization of the following novel compounds: aculen A-D, aculabistrins A-B, acu-dioxomorpholine, okaramine S, and epi-10,23-dihydro-24,25-dehydroaflavinin from A. aculeatus, aspiperidine oxide from A. indologenous, homomorphosins A-F from A. homomorphus, sclerotionigrins A-B from A. sclerotioniger, as well as emindole SC, sclerolizine and carbonaranis I-J from A. sclerotii-carbonarius. In addition, several known compounds could be reported from the different species for the first time. Furthermore it was discovered how sclerotia formation could be induced in black Aspergilli, using a combination of natural substrates and by introduction of a pre-freezing step prior to inoculation. This is of general interest for the discovery of novel bioactive SMs, since sclerotia formation trigger otherwise silent biosynthetic pathways, resulting in greatly altered metabolic profiles.
The second part of the study, linking genes to SMs and elucidating biosynthetic pathways, led to insights into the biosynthetic potential of a number of Aspergilli. This included comparative metabolic profiling of A. oryzae and A. flavus,
two species with an overall high homology of 99.5 % on genome level, but surprisingly high degree of chemical
differences. Elucidation of structures from novel A. oryzae metabolites, however, revealed the chemical link between the
two species. In two parallel projects, involving A. niger and A. aculeatus respectively, the polyketide 6-methyl salicylic acid
(6-MSA), and corresponding biosynthetic pathways, were investigated. In A. niger, 6-MSA was converted into
meroterpenoid yanuthone D. The biosynthetic pathway was investigated by a multidisciplinary approach. As a result the
cluster responsible for production of yanuthone D was identified and a biosynthetic pathway presented, where 6-MSA is
converted into yanuthone D in eight steps. Furthermore a total of ten novel yanuthones were characterized, whereof two
did not originate from 6-MSA, but did utilize several of the enzymes encoded by the cluster, defining a new class of
yanuthones. In A. aculeatus the 6-MSA pathway was found to differ, with conversion of 6-MSA into the terpenoid/non-
ribosomal peptide/polyketide hybrids aculins A-B, for which a biosynthetic pathway has been proposed. By overexpression
of a TF located immediately downstream of the 6-MSA synthase gene, two non-6-MSA derived compounds were
additional discovered. In A. nidulans a supercluster consisting of a non-ribosomal peptide synthase and a
prenyltransferase was predicted, by full genome gene expression comparison, which ultimately linked to the
tetracyclopeptide nidulanin A, illustrating the strength of bioinformatic tools to predict superclusters and structures of
NRPs. Finally, it was investigated how entire gene clusters from filamentous fungi could be reconstituted in the
model organism A. nidulans. This project would improve discovery, and ease characterization, of genes. As proof of
concept, the cytochalasin gene cluster from A. clavatus was successfully reconstituted in A. nidulans, allowing further
biochemical characterization.

The work of this thesis represents a major step forward in extending the chemical knowledge on the complex secondary
metabolism of important filamentous fungi and at the same time illustrates the enormous potential for still discovering
novel SMs. A focused collaboration between bioinformatics, molecular biology, analytical and natural products chemistry is
critical for advances in both the linking of fungal SMs to genes and unraveling the biosynthetic pathways, as well as for the
discovery of novel SMs hidden in a treasury of biosynthetic potential of filamentous fungi.

General information
State: Published
Organisations: Department of Systems Biology, Department of Chemistry, Organic Chemistry, Eucaryotic Molecular Cell
Biology
Authors: Petersen, L. M. (Intern), Larsen, T. O. (Intern), Gotfredsen, C. H. (Intern), Nielsen, J. B. (Intern)
Number of pages: 471
Publication date: 2014

Publication information
Publisher: Department of Systems Biology, Technical University of Denmark
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
Linking_fungal_secondary_metabolites.pdf

Relations
Projects:
Linking fungal secondary metabolites and pathways to their genes in Aspergillus
Publication: Research › Ph.D. thesis – Annual report year: 2016

Low-Temperature NH3–SCR of NO on Mesoporous Mn0.6Fe0.4/TiO2 Prepared by a Hydrothermal Method
Mesoporous 30 wt% Mn0.6Fe0.4/TiO2 has been prepared by a novel hydrothermal method using a structure directing
agent and characterized by N2 adsorption, SEM, XRD, EDX, H2-TPR and the catalytic activity for the selective catalytic
reduction (SCR) of NO by ammonia was measured under power plant flue gas conditions. Compared to 30 wt%
Mn0.6Fe0.4/TiO2 prepared by impregnation, the average pore size was significantly increased. The method of preparation
has only a small effect on the catalytic activity at temperatures between 125 and 300 °C. The hydrothermal preparation
method leads to a somewhat higher (NH4)2SO4 tolerance at 150 °C compared to the impregnation preparation method.
Regeneration of the (NH4)2SO4 loaded samples by heating to 400 °C was not possible whereas water washing yielded
better regeneration. The catalysts are significantly more active than a commercial VWT SCR catalyst at temperatures up
to 200 °C, but do not match the activity of the latter at the higher temperatures typically encountered at the high dust
position in power plants.

General information
State: Published
Organisations: Centre for Catalysis and Sustainable Chemistry, Department of Chemistry, Department of Chemical and
Biochemical Engineering, CHEC Research Centre
Authors: Schill, L. (Intern), Putluru, S. S. R. (Intern), Fehrmann, R. (Intern), Jensen, A. D. (Intern)
Pages: 395-402
Publication date: 2014
Main Research Area: Technical/natural sciences
Lysine Glutarylation Is a Protein Posttranslational Modification Regulated by SIRT5

We report the identification and characterization of a five-carbon protein posttranslational modification (PTM) called lysine glutarylation (Kglu). This protein modification was detected by immunoblot and mass spectrometry (MS), and then comprehensively validated by chemical and biochemical methods. We demonstrated that the previously annotated deacetylase, sirtuin 5 (SIRT5), is a lysine deglutarylase. Proteome-wide analysis identified 683 Kglu sites in 191 proteins and showed that Kglu is highly enriched on metabolic enzymes and mitochondrial proteins. We validated carbamoyl phosphate synthase 1 (CPS1), the rate-limiting enzyme in urea cycle, as a glutarylated protein and demonstrated that CPS1 is targeted by SIRT5 for deglutarylation. We further showed that glutarylation suppresses CPS1 enzymatic activity in cell lines, mice, and a model of glutaric acidemia type I disease, the last of which has elevated glutaric acid and glutaryl-CoA. This study expands the landscape of lysine acyl modifications and increases our understanding of the deacylase SIRT5.

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry, University of Chicago, Duke University, University of Michigan, University Medical Center Hamburg-Eppendorf, US National Institute of Health, Chinese Academy of Sciences, University of Colorado
Pages: 605-617
Publication date: 2014
Main Research Area: Technical/natural sciences

Publication information
Journal: Cell Metabolism
Volume: 19
Issue number: 4
ISSN (Print): 1550-4131
Ratings:
BFI (2018): BFI-level 3
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 13.19 SJR 11.209 SNIP 2.941
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 11.801 SNIP 3.024 CiteScore 13.39
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 11.468 SNIP 2.947 CiteScore 13.34
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 10.215 SNIP 2.9 CiteScore 12.23
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 8.911 SNIP 2.917 CiteScore 11.03
ISI indexed (2012): ISI indexed yes
Metal-catalyzed variations on the Pictet-Spengler theme

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry
Authors: Hansen, C. L. (Intern), Ascic, E. (Intern), Le Quement, S. T. (Intern), Nielsen, T. E. (Intern)
Publication date: 2014
Conference: 245th National Spring Meeting of the American-Chemical-Society, New Orleans, LA, United States, 07/04/2013 - 07/04/2013
Main Research Area: Technical/natural sciences

Publication information
Journal: Abstracts of Papers of the American Chemical Society
Volume: 245
Article number: 831-ORGN
ISSN (Print): 0065-7727
Ratings:
Web of Science (2018): Indexed yes
Web of Science (2017): Indexed Yes
Scopus rating (2014): SJR 0.101 SNIP 0.013
Web of Science (2014): Indexed yes
Scopus rating (2013): SJR 0.101 SNIP 0.003
Web of Science (2013): Indexed yes
Scopus rating (2012): SJR 0.1 SNIP 0
Scopus rating (2011): SJR 0.101 SNIP 0
Web of Science (2011): Indexed yes
Scopus rating (2010): SJR 0.101 SNIP 0
Scopus rating (2009): SJR 0.101 SNIP 0
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.101 SNIP 0
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.101 SNIP 0
Scopus rating (2006): SJR 0.101
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.101
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.104 SNIP 0.028
Web of Science (2004): Indexed yes
Methyl 1-ethyl-3'-[hydroxy(naphthalen-1-yl)methyl]-1'-methyl-2-oxospiro[indoline-3,2'-pyrrolidine]-3'-carboxylate

In the title compound, C27H28N2O4, the pyrrolidine ring adopts a twist conformation. The plane of the indole ring is almost perpendicular to that of the pyrrolidine ring, making a dihedral angle of 88.50(6)°. The planes of the naphthyl ring system and the pyrrolidine ring are tilted by an angle of 55.86(5)°. The molecular conformation is stabilized by intramolecular O - H⋯O and O - H⋯N hydrogen bonds. © 2014 CrossMark.

General information
State: Published
Organisations: Department of Chemistry, Physical and Biophysical Chemistry, Roskilde University, University of Madras, Presidency College, Chennai
Authors: Vijayakuma, V. (Ekstern), Peters, G. H. (Intern), Suresh, C. (Ekstern), Raghavachary, R. (Ekstern), Jagadeesan, G. (Ekstern)
Number of pages: 10
Publication date: 2014
Main Research Area: Technical/natural sciences

Publication information
Journal: Acta Crystallographica. Section E: Structure Reports Online
Volume: 70
Issue number: 5
Article number: o540
ISSN (Print): 1600-5368
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
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
Methyl Effect in Azumamides Provides Insight Into Histone Deacetylase Inhibition by Macrocycles

Natural, nonribosomal cyclotetrapeptides have traditionally been a rich source of inspiration for design of potent histone deacetylase (HDAC) inhibitors. We recently disclosed the total synthesis and full HDAC profiling of the naturally occurring azumamides (J. Med. Chem. 2013, 56, 6512). In this work, we investigate the structural requirements for potent HDAC inhibition by macrocyclic peptides using the azumamides along with a series of unnatural analogues obtained through chemical synthesis. By solving solution NMR structures of selected macrocycles and combining these findings with molecular modeling, we pinpoint crucial enzyme–ligand interactions required for potent inhibition of HDAC3. Docking of additional natural products confirmed these features to be generally important. Combined with the structural conservation across HDACs 1–3, this suggests that while cyclotetrapeptides have provided potent and class-selective HDAC inhibitors, it will be challenging to distinguish between the three major class I deacetylases using these chemotypes.

General information
State: Published
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Scopus rating (2016): CiteScore 6.06
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Scopus rating (2015): SJR 2.529 SNIP 1.631 CiteScore 5.66
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Scopus rating (2014): SJR 2.259 SNIP 1.693 CiteScore 5.55
Mo- and V-catalyzed transformation of biomass into high-value chemicals

The possibility of converting biomass into higher-value chemicals has received increased attention over the last few years. If biomass could be converted into biofuels or platform chemicals, then it could constitute a large source of renewable energy and economy for society.

General information

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Organisations: Department of Chemistry, Organic Chemistry
Authors: Nielsen, L. B. (Intern), Dethlefsen, J. R. (Intern), Lupp, D. (Intern), Fristrup, P. (Intern)
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Molecular and Chemical Characterization of the Biosynthesis of the 6-MSA-Derived Meroterpenoid Yanuthone D in Aspergillus niger.

Secondary metabolites in filamentous fungi constitute a rich source of bioactive molecules. We have deduced the genetic and biosynthetic pathway of the antibiotic yanuthone D from Aspergillus niger. Our analyses show that yanuthone D is a meroterpenoid derived from the polyketide 6-methylsalicylic acid (6-MSA). Yanuthone D formation depends on a cluster composed of ten genes including yanA and yanI, which encode a 6-MSA polyketide synthase and a previously undescribed O-mevalon transferase, respectively. In addition, several branching points in the pathway were discovered, revealing five yanuthones (F, G, H, I, and J). Furthermore, we have identified another compound (yanuthone X1) that defines a class of yanuthones that depend on several enzymatic activities encoded by genes in the yan cluster but that are not derived from 6-MSA.

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BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 5.43 SJR 3.201 SNIP 1.301
Scopus rating (2015): SJR 3.192 SNIP 1.416
Scopus rating (2014): SJR 3 SNIP 1.385
Web of Science (2014): Indexed yes
Scopus rating (2013): SJR 2.988 SNIP 1.359
ISI indexed (2013): ISI indexed yes
Scopus rating (2012): SJR 2.787 SNIP 1.302
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
Scopus rating (2011): SJR 2.861 SNIP 1.394
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
Scopus rating (2010): SJR 2.786 SNIP 1.319
Web of Science (2010): Indexed yes
Scopus rating (2009): SJR 2.885 SNIP 1.464
Scopus rating (2008): SJR 2.483 SNIP 1.273
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 2.761 SNIP 1.355
Scopus rating (2006): SJR 2.57 SNIP 1.364
Scopus rating (2005): SJR 2.644 SNIP 1.421
Scopus rating (2004): SJR 2.758 SNIP 1.424
Scopus rating (2003): SJR 3.046 SNIP 1.558
Scopus rating (2002): SJR 3.015 SNIP 1.59
Scopus rating (2001): SJR 3.081 SNIP 1.475
Scopus rating (2000): SJR 4.008 SNIP 1.553
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Molybdenum-catalyzed deoxydehydration of vicinal diols

The commercially available (NH₄)₆Mo₇O₂₄ and other molybdenum compounds are shown to be viable substitutes for the typically employed rhenium compounds in the catalytic deoxydehydration of aliphatic diols into the corresponding alkenes. The transformation, which represents a model system for the various hydroxyl groups found in biomass-derived carbohydrates, can be conducted in an inert solvent (dodecane), under solvent-free conditions, and in a solvent capable of dissolving biomass-derived polyols (1,5-pentanediol). The reaction is driven by the simultaneous oxidative deformylation of the diol resulting in an overall disproportionation of the substrate.

General information

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Organisations: Department of Chemistry, Organic Chemistry, Technical University of Denmark
Authors: Dethlefsen, J. R. (Intern), Lupp, D. (Intern), Oh, B. C. (Ekstern), Fristrup, P. (Intern)
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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
Scopus rating (2011): SJR 2.767 SNIP 1.504 CiteScore 5.53
ISI indexed (2011): ISI indexed no
Web of Science (2011): Indexed yes
Scopus rating (2010): SJR 1.945 SNIP 1.134
Web of Science (2010): Indexed yes
Scopus rating (2009): SJR 0.973 SNIP 0.72
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.291 SNIP 0.48
Web of Science (2008): Indexed yes
Nanoporous gold assembly of glucose oxidase for electrochemical biosensing

Nanoporous gold (NPG) is composed of three-dimensional (3D) bicontinuous nanostructures with large surface area. Nano-channels inside NPG provide an ideal local environment for immobilization of enzyme molecules with expected stabilization of the protein molecules. In this work, glucose oxidase (GOx) has been brought to assemble on NPG via surface chemical reactions to form enzyme modified NPG nanomaterial with promising sensitivity for glucose detection. Cyclic voltammetry and single-potential step chronoamperometry (SPSC) are employed to study the electrochemical behavior of both bare and enzyme-modified NPG. Two redox mediators, p-benzoquinone (BQ) and ferrocenecarboxylic acid (FCA) are used to shuttle electrons between the enzyme redox center inside of GOx and the NPG electrode. Diffusion patterns at the functionalized NPG electrode are found significantly different from those on planar gold electrodes. This is mainly caused by internal 3D single crystal-like structures of NPG. Electrostatically neutral BQ mediator gives much higher voltammetric sensitivity than negatively charged FCA for GOx modified NPG electrodes. This study provides insight into the understanding of the intrinsic properties of NPG materials aiming at evolving enzymatic biosensors with high performance. © 2014 Elsevier Ltd.

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Organisations: Department of Chemistry, NanoChemistry, Shandong University
Authors: Xiao, X. (Ekstern), Ulstrup, J. (Intern), Li, H. (Ekstern), Wang, M. (Ekstern), Zhang, J. (Intern), Si, P. (Forskerdatabase)
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Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
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Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.435 SNIP 1.607 CiteScore 4.44
Nanoscale Electrocatlyst for Chemical and Biological Sensor

This dissertation describes scientific research that covers preparation and use of two classes of designed inorganic hybrid nanostructures (nanoparticles and graphene) as electrocatalysts in interfacial molecular and biomolecular electron transfer and electrocatalysis. Emphasis is on both fundamental properties of the nanostructures and on their use in chemical and biological sensing devices at the single-molecular scale. The project is focused on electroactive (or redox) Prussian blue nanoparticles (PBNPs) as well as on graphene and quantum dots (QDs). The results have offered significant interests in understanding of fundamental electronic properties of hybrid nanomaterials and their potential applications in next generation ultra-sensitive chemical sensors and biosensors. As the first man-made coordination compound, Prussian Blue (PB) has a long history dating back over 300 years ago (the first synthesis in 1704). This interesting material has recently been used broadly as an electron transfer (ET) catalyst for new chemical and biological sensors. We have initiated efforts in synthesis, functional characterization and applications of PB in novel nanostructured forms focused on controlled-size PB nanoparticles (PBNPs). Fast and reversible interfacial PBNP ET on an Au (111) electrode surface modified with
Functional alkanethiols was detected. In terms of ET characteristics, assembled on a solid surface in a two-dimensional array these nanoparticles behave like a large redox molecule such as a metalloenzyme in the electrocatalytic reduction of H₂O₂ and glucose oxidation, suggesting a tunneling mechanism. Furthermore, the interfacial electrochemical ET and electrocatalysis of PBNPs immobilized on Au(111)-electrode surfaces modified by variable-length differently functionalized thiol-based self-assembled molecular monolayers (SAMs) have been explored. The SAMs are terminated by positively (-NH₃⁺) and negatively charged groups (-COO⁻) as well as by neutral hydrophobic groups (-CH₃). In addition, three-dimensional networks of cross-linked [Poly(ethylenimine) (PEI)] onto which PBNPs are attached by electrostatic forces have been fabricated and assembled on single-crystal Au(111) electrode surfaces to enhance electrocatalysis resulting from the 3D nanostructure skeleton. In situ AFM of the different assembled layers in the electrolyte solution shows molecular scale structures on the surface, in keeping with electrochemical behavior. To increase the conductivity of PBNPs as an active electrode, reduced graphene oxide (RGO) and PBNPs were exploited as building ingredients to prepare with increased electrical conductivity and functional variability nanohybrid electrocatalysts, which are further transformed into free-standing graphene papers. PBNPs doped graphene paper shows highly efficient electrocatalysis towards reduction of hydrogen peroxide and can be used as flexible chemical sensors for potential applications in detection of hydrogen peroxide or/and other organic peroxides. The as-prepared PBNPs-RGO paper is further capable of biocompatible accommodation of enzymes for development of freestanding enzyme based biosensors and as a potentially platform for electrocatalytic energy conversion. Graphene/PBNPs paper obtained using Au filter substrate shows high electrical conductivity, outstanding mechanical strength, excellent thermal stability, and structural uniformity. This type of paper has good electrochemical performance. Strong electrocatalysis property has, furthermore, been achieved using these mixed materials. This variety of flexible active electrodes can be freely used for electrocatalytic monitoring H₂O₂, glucose or other analytes. A new method based on one-step oil/water (O/W) two phase induced interfacial self-assembly of RGO nanosheets into graphene nanofilms has been refined. The method shows high efficiency for incorporation of CdSe quantum dots (QDs) into nanofilms to prepare QDs doped graphene nanostructures. Confined QDs interact closely with RGO to promote and to significantly enhance photoinduced electron or energy transfer between RGO and CdSe QDs, which could hold promise for their applications as photovoltaic materials in solar cells.

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Organisations: Department of Chemistry

Authors: Zhu, N. (Intern), Chi, Q. (Intern), Ulstrup, J. (Intern)

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**Negative Flash for Calculating the Intersecting Key Tie lines in Multicomponent Gas Injection**

Gas injection is a widely used enhanced oil recovery method, and its application is expected to increase in the foreseeable future. In order to build a method of characteristics solution to a two-phase gas injection system, we must construct the composition route from the injection gas to the initial oil where all the intersecting key tie lines must be identified. Calculation of these intersecting tie lines requires a series of special negative flashes, which allow not only phase fractions outside the physical interval [0,1] but also negative feed compositions. The phase compositions from one negative flash are used to recombine the feed for the next negative flash. Despite the apparent complexity due to multicomponent phase equilibrium and transport, for pure component gas injection, negative flash and elimination of components can be performed in an alternating manner. In particular, if K-values are constant, there exists a simple feature that the vapor fraction roots (beta-roots) for the RachfordRice equation for the initial oil are the roots to be found in all the negative flashes involved. This leads to a simple and well-structured algorithm for the solution with constant K-values. A special problem with pure component gas injection is that there could be two possible roots in the beta-interval of interest. But if the component to be eliminated is left with an infinitesimal amount due to the diffusion or dispersion effects, only the larger root can still give non-negative phase compositions and should thus be selected. For multicomponent gas injection with constant K-values, the vapor fraction roots in all the involved negative flashes are simply from the vapor fraction roots for the initial oil (beta-roots) and those for the injection gas (lambda-roots). By solving just two negative flashes for the initial oil and the injection gas and using proper selection sequences for these beta- and lambda-roots, we can readily determine all the intersecting tie lines for constant K-values.
NiO/YSZ Reduction for SOFC/SOEC Studied In Situ by Environmental Transmission Electron Microscopy

SOFCs/SOECs are typically composed of ceramic materials, which are highly complex at the nano-scale. Scanning and transmission electron microscopy (SEM and TEM) are routinely applied for studying these nano-scaled structures post mortem, but only few SOFC/SOEC studies have applied environmental TEM (ETEM). ETEM offer the possibility to record image series (movies) of the ceramic nanostructures with atomic scale resolution during exposure to a reactive gas environment at elevated temperatures. The present contribution focuses on the typical reduction preparation step for the state-of-the-art Ni/YSZ (YSZ = Y2O3-stabilized ZrO2) based anodes for SOFC and cathodes for SOEC. Specifically, the reduction of nickel oxide to form the catalytically active nickel surface is monitored directly at the nano- and atomic scale by using an ETEM. The reduction process was followed while exposing NiO/YSZ and pure NiO to H2 at temperatures from room temperature to ca. 800°C. The NiO/YSZ was prepared by crushing down a tape casted and sintered model anode/cathode into a fine powder. Previous studies based on averaging techniques have shown that the reduction of pure NiO is a relatively rapid process, while the reduction of NiO/YSZ is slower, which indicates that the presence of YSZ inhibits the reduction of NiO. In the presents in situ experiments the temperature dependent reduction profile are found similar for the both nano-scaled NiO and NiO/YSZ sample. The apparent inhibitive effect of YSZ on NiO reduction is therefore not caused by a direct interaction between NiO and YSZ, but is an indirect effect depending on the NiO being integrated in a macroscopic network of NiO/YSZ. A Titan E-Cell 80-300ST TEM was used for the in situ work in combination with the chip-based heating holder from Protochips which facilitated rapid temperature ramping for example from room temperature to 800°C in only 1 s. The ETEM results are compared to complementary averaging techniques such as thermo-gravimetric analysis (TGA) and X-ray diffraction analysis (XRD). The figure presents a TEM image series of NiO during exposure to 2 mbar H2 and constant temperature ramping rate of 1°C/min. The NiO observed in the first image at 320°C is dense. From the lower left corner a front of porous Ni is progressing until full reduction at 340°C. [Formula]
NiO/YSZ Reduction for SOFC/SOEC Studied In Situ by Environmental Transmission Electron Microscopy

A typical anode for solid oxide fuel cells (SOFC) or cathode for solid oxide electrolysis cells (SOEC) is a complex porous structure of Ni and yttria-stabilized zirconia (YSZ). The porous Ni/YSZ is usually prepared from powder mixtures of NiO and YSZ, tape casted and sintered into a dense structure and finally reduced during start-up of the SOFC/SOEC in H2 at the operating temperature of the cell (ca. 800 °C). This contribution presents environmental transmission electron microscopy (ETEM) nanoscale observations of the reduction process of a NiO/YSZ powder in H2 at temperatures up to almost 1000 °C. The study focusses on the temperature dependent dynamical morphology of the NiO/YSZ and on the possible influence of YSZ on the NiO reduction.

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BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.214 SNIP 0.246 CiteScore 0.36
BFI (2013): BFI-level 1
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ISI indexed (2013): ISI indexed no
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ISI indexed (2011): ISI indexed no
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BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.241 SNIP 0.266
BFI (2008): BFI-level 1
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NMR structural studies of oligosaccharides and other natural products

NMR spectroscopy is an important tool in chemical analysis and for structural studies in various research areas. The subject of this thesis is liquid state NMR spectroscopy for structural analysis of small molecules, both regarding method development and structure elucidation by NMR spectroscopy.

HMBC+ is a new pseudo-3D NMR experiment for measurement of long-range homonuclear JHH coupling constants in small molecules. Based on two existing experiments, multiplicity edited HMBC and HAT HMBC by Benie, Nyberg, and Sørensen, the new HMBC+ experiment takes advantage of a π phase difference with respect to n+1JHH between these two experiments, observed in the nJCH HMBC cross peak. Through a double editing procedure this enables straightforward determination of both sign and magnitude of n+1JHH, including for very small coupling constants.

Excellent results were obtained for the natural product strychnine, and 28 n+1JHH coupling constants were determined, of which 10 had not previously been measured due to their small sizes. By comparing to calculated coupling constants, an RMSD of 0.28 Hz was obtained, all coupling constant signs fit with the calculations, and all errors were below 1 Hz, also when comparing the absolute values to experimental coupling constants measured by Carter et al. using 1D 1H NMR on deuterated strychnine analogues. Providing an excellent tool for measurement of long-range JHH with the extra convenience of labeling the coupling constant information to the 13C chemical shift through the nJCH correlation, this experiment has exciting applications for configurational assignment of e.g. carbohydrates and for residual dipolar couplings.

Identification of known molecules and discovery of novel molecules are other important applications of NMR spectroscopy. Bacteria and fungi produce secondary metabolites for signaling and competing against other organisms, and these molecules are important in drug discovery due to their inherent biological activities. From a marine Photobacterium (P. halotolerans) we isolated the solonamides and the ngercheumicins, two families of cyclic depsipeptides capable of attenuating virulence in S. aureus by quorum sensing inhibition through the accessory gene regulator agr. This is likely due to their structural similarities with the auto-inducing peptides of S. aureus, controlling quorum sensing in bacterial populations. A filamentous fungus, A. fijiensis, was also investigated for production of novel secondary metabolites, and a new pyranonigrin (E) was isolated and structure elucidated by NMR spectroscopy along with JBIR-74 and decumbenone A, two known metabolites previously isolated from Aspergillus and Penicillium species.

Oligosaccharides found in human milk are important for infant nutrition, and a collaborative effort of university and industry partners was aimed at establishing methods for production of human milk oligosaccharides. Two different bioenzymatic methods for production of 3'-sialyllactose were investigated, and a screening of trans-fucosidases enabled the NMR spectroscopic identification of three pNP-fucosylfucopyranosides as major reaction products.

Novel 4-component reaction for the synthesis of boron heterocyclic scaffolds

General information
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Organisations: Department of Chemistry, Organic Chemistry
Authors: Petersen, M. T. (Intern), Flagstad, T. (Intern), Nielsen, T. E. (Intern)
Publication date: 2014
One-pot glycosylations in the synthesis of human milk oligosaccharides

Human milk oligosaccharides contain a well-defined core structure that makes them interesting synthetic targets for one-pot glycosylation strategies. In this investigation, a one-pot procedure was studied in which a galactose thioglycoside is coupled chemoselectively to a phthalimide-protected glucosamine thioglycoside, and the resulting disaccharide is then coupled to the 3'-position in lactose. Very high yields of the tetrasaccharide product can be obtained when a protected lactosamine thioglycoside is formed in the first coupling. In contrast, it was not possible to extend the one-pot process to the synthesis of the corresponding 3″-linked structures, due to an inefficient synthesis of the lacto-N-biose thioglycoside in the first glycosylation. This is explained by the reactivity difference between the 3- and 4-positions in phthalimide-protected glucosamine. The one-pot procedure has been applied in an efficient synthesis of the pentasaccharide lacto-N-neofucopentaose I, which is composed of N-acetyllactosamine, lactose, and fucose. On the other hand, a stepwise approach was found to be the preferred synthetic pathway for preparation of the isomeric lacto-N-fucopentaose I, which contains a lacto-N-biose moiety.

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Scopus rating (2016): CiteScore 2.74 SJR 1.133 SNIP 0.653
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.198 SNIP 0.758 CiteScore 2.88
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.181 SNIP 0.767 CiteScore 2.96
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.292 SNIP 0.796 CiteScore 2.96
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.471 SNIP 0.811 CiteScore 2.93
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.536 SNIP 0.857 CiteScore 3.2
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.572 SNIP 0.785
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.497 SNIP 0.778
Web of Science (2009): Indexed yes
On petroleum fluid characterization with the PC-SAFT equation of state

The perturbed-chain statistical associating fluid theory (PC-SAFT) equation of state has shown promising results for describing complex phase behaviors and high pressure properties of various systems. It has been proposed as an alternative to the classical cubic equations of state in the petroleum industry. It is, however, far from a simple task to develop a sophisticated oil characterization method for the PC-SAFT EOS. In this work, in order to answer some fundamental questions of developing new characterization methods for PC-SAFT, six methods are proposed to estimate the model parameters by combining the well-behaved correlations of homologous series with the PNA contents and/or by using different fitting approaches. Along with different options in characterization procedure, the performance of these methods is investigated on PVT calculations, i.e. predicting the saturation pressure and density of 80 petroleum fluids over wide temperature, pressure and composition conditions. These options include the molar composition distribution, the specific gravity correlation, the number of pseudo-components, the estimation method of PNA contents and the binary interaction parameters. Two candidate methods are showing better overall performance than the others, with deviations less than 6.0% and 1.3% of saturation pressure and density, respectively. These two methods are further studied for predicting more complete sets of PVT data, i.e. constant mass expansion, differential liberation and separator test, of three petroleum fluids. The results are promising if compared to those available in the literature. © 2014 Elsevier B.V.
On solving the Rachford-Rice equation with higher order methods

The Rachford-Rice equation calculates the amounts and compositions of two equilibrium phases at constant K-factors. This single variable equation is a perfect candidate for applying higher order iteration methods because the additional cost for evaluating the derivatives with order higher than two is relatively low. This study compares the performance of Householder's high order iterations up to order seven. In addition, a method to improve the initial estimate is proposed for the situation where the Rachford-Rice function shows abrupt change close to the asymptotes and overshooting happens. The proposed method can largely reduce repeated use of the bisection adjustment in the subsequent iterations. The comparison shows that the Householder's iteration with order three or four gives the best performance on average.

General information
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Authors: Yan, W. (Intern), Stenby, E. H. (Intern)
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Scopus rating (2016): CiteScore 2.33 SJR 0.869 SNIP 1.155
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.874 SNIP 0.998 CiteScore 1.99
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 0.982 SNIP 1.248 CiteScore 2.28
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BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.007 SNIP 1.274 CiteScore 2.31
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.152 SNIP 1.286 CiteScore 2.31
ISI indexed (2012): ISI indexed yes
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BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.034 SNIP 1.234 CiteScore 2.26
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
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Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.133 SNIP 1.164
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.227 SNIP 1.09
On the development of quality assurance

Contemporary research in quality assurance indicates that large uncertainties observed in interlaboratory comparisons to a large extent originate from a lack of competence of laboratory staff. This explanation is challenged by the present article for which six technologies and multiple series of experiments were investigated with respect to uncertainty of measurement and treatment of outliers. It was found that long-term precision was poor in comparison to short-term precision. The ratio of predicted uncertainty to observed uncertainty was determined as significantly above 1, and it was suggested that a correction factor is needed for the predicted uncertainty. This indicates that statistical control could be obtained only by treating many independent series of experiments and using pooled calibrations in the method validation. Retention of outliers in calculation of contents and calculation of uncertainties of certified reference materials (CRMs) gave results that differed significantly from those in the certificates of the CRMs. (C) 2014 Elsevier B.V. All rights reserved.
On the freezing behavior and diffusion of water in proximity to single-supported zwitterionic and anionic bilayer lipid membranes

We compare the freezing/melting behavior of water hydrating single-supported bilayers of a zwitterionic lipid DMPC with that of an anionic lipid DMPG. For both membranes, the temperature dependence of the elastically scattered neutron
intensity indicates distinct water types undergoing translational diffusion: bulk-like water probably located above the membrane and two types of confined water closer to the lipid head groups. The membranes differ in the greater width of the water freezing transition near the anionic DMPG bilayer compared to zwitterionic DMPC as well as in the abruptness of the freezing/melting transitions of the bulk-like water. © CopyrightEPLA, 2014.

General information
State: Published
Organisations: Department of Chemistry, University of Missouri, University of Maryland, Oak Ridge National Laboratory
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Main Research Area: Technical/natural sciences

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BFI (2018): BFI-level 2
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BFI (2017): BFI-level 2
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Scopus rating (2016): CiteScore 1.18 SJR 0.523 SNIP 0.597
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.584 SNIP 0.628 CiteScore 1.12
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 0.547 SNIP 0.593 CiteScore 1.04
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 0.537 SNIP 0.54 CiteScore 1
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 0.809 SNIP 0.606 CiteScore 1.28
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.386 SNIP 0.767 CiteScore 1.86
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.782 SNIP 0.769
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.024 SNIP 0.973
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.778 SNIP 1.034
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.961 SNIP 1.062
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.878 SNIP 1.032
Organometallic Methods for Forming and Cleaving Carbon-Carbon Bonds

The retro-Grignard addition reaction has been revisited and the benzyl addition reaction was found to be a reversible transformation by using crossover experiments. The retro benzyl addition reaction was shown by the addition of benzylmagnesium chloride to di-t-butyl ketone followed by exchange of both the benzyl and the ketone moiety with another substrate. Similar experiments were performed with phenylmagnesium bromide and t-butylmagnesium chloride, but in these two cases the Grignard addition reaction did not show any sign of a reverse transformation.

The ring-opening of cyclic ethers with concomitant C-C bond formation was studied with a number of Grignard reagents. The transformation was performed in a sealed vial by heating to about 160 °C in an aluminum block or at 180 °C in a microwave oven. Good yields of the product alcohols were obtained with allyl- and benzylmagnesium halides when the ether was tetrahydrofuran or 3,3-dimethyloxetane. Lower yields were obtained with substituted tetrahydrofurans while no ring-opening was observed with tetrahydropyran. Only highly reactive allyland benzylmagnesium halides participated in the transformation while no reaction occurred with other alkylmagnesium halides.

Carbohydrates with protecting groups on all alcohol groups except the primary alcohol were prepared and subjected to the iridium catalyzed dehydrogenative decarbonylation reaction where primary alcohols are converted into the corresponding one carbon shorter products. Modest conversions were obtained when isopropylidene- or cyclohexylidene ketals were used as protecting groups, but the conversion rate was slow. Low conversion was obtained when the alcohols were protected by benzyl groups and the carbohydrates were unstable at the required temperatures. The syngas evolved from the iridium catalyzed dehydrogenative decarbonylation reaction was consumed in a palladium catalyzed reductive carbonylation reaction in a two-chamber system setup. Carbohydrates were not found to be a viable syngas source because they did not liberate sufficient syngas. Carbohydrates were attached to several lipophilic anchors and performing the dehydrogenative decarbonylation with the anchor monools proceeded well, while the corresponding anchor triols were unstable at the elevated temperatures. Of the simple primary alcohols investigated, 2-(2-naphthyl)ethanol, hexane-1,6-diol and dodecane-1,12-diol were found to be the most promising syngas sources. A substrate scope for the reductive carbonylation of aryl bromides is currently under development by using hexane-1,6-diol as a syngas source.

The synthesis of the anticancer antibiotic tetrahydroisoquinoline alkaloid jorumycin progressed via a route consisting of a crucial aryne annulation step where an isoquinoline scaffold was prepared. The aryne annulation step was problematic and after several attempted modifications to the formerly optimized procedure; no further improvement was obtained. Gratifyingly, an alternative route was found for the formation of the isoquinoline scaffold and further optimization of this route is needed.
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.

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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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BFI (2012): BFI-level 1
ISI indexed (2012): ISI indexed no
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
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BFI (2010): BFI-level 1
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BFI (2008): BFI-level 1
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Original language: English
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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 606molacetaldehyde/molAu.hour⁻¹.
Oxygen evolution catalysts on supports with a 3-D ordered array structure and intrinsic proton conductivity for proton exchange membrane steam electrolysis

Proton exchange membrane steam electrolyzers suffer from insufficient catalyst activity and durability due to the slow reaction kinetics for oxygen evolution reaction (OER) and poor durability under harsh operating environments. Aiming at enhancement of oxygen electrode kinetics and durability, composite support materials for iridium oxide are synthesized via in situ phosphorization reaction on tin doped indium oxide and possess functionalities of high electronic and intrinsic proton conductivity. At 130 °C under a water vapor atmosphere an overall conductivity of 0.72 S cm−1 is achieved with a contribution of around 10−2 S cm−1 proton conductivity. The support structure of three-dimensionally ordered hexagonal arrays displays a high specific surface area of 180 m² g−1. Benefiting from the mixed conductivities and porous structure in the composite support materials, the supported IrO₂ catalysts exhibit about five times enhancement of the OER activity in acidic electrolytes. The improved catalytic performance for the OER was further confirmed by PEM electrolyzer tests at 130 °C. A test of such a steam electrolyzer cell at 350 mA cm⁻² shows good durability within a period of up to 1150 hours.

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Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Brønsted acid ionic liquids (BAILs) were prepared and applied as combined acid promoters and reaction media in Pd–phosphine catalyzed methoxycarbonylation of ethylene to produce methyl propionate. The BAILs served as alternatives to common mineral acids required for the reaction, e.g. methanesulfonic acid or sulfuric acid, resulting in high catalytic activity and selectivity towards methyl propionate. In addition, the BAILs yielded a biphasic system with the product and provided stability to palladium intermediates avoiding the undesirable formation of palladium black after reaction. These special features enabled facile methyl propionate separation and recovery of the ionic liquid catalyst system, thus allowing its re-use up to 15 times without apparent loss of catalytic activity or selectivity.

**General information**

**State:** Published

**Organisations:** Department of Chemistry, Centre for Catalysis and Sustainable Chemistry

**Authors:** Garcia-Suarez, E. J. (Intern), Khokarale, S. G. (Intern), Nguyen van Buu, O. (Intern), Fehrmann, R. (Intern), Riisager, A. (Intern)

**Pages:** 161-166

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Petasis-type reactions for the synthesis of substituted pyrrolidin-2-ones

Pyrrolidin-2-ones are important heterocyclic motifs found in natural products and biologically active synthetic molecules. Addition of nucleophiles, including allylsilanes, isonitriles and organometallics, to N-acyliminium ions represents one of the most commonly used approaches for the formation of substituted pyrrolidin-2-ones. Only few studies on the nucleophilic addition of organoboronic acids to N-acyliminium ions have been reported. Herein, we disclose our recent efforts for the synthesis of substituted pyrrolidin-2-ones through Lewis-acid-mediated Petasis-type reactions. By implementing a reductive cyclization reaction, linear L-malic acid derivatives were rapidly converted into cyclic N-acyliminium ions. Under the optimized conditions, entailing the use of HFIP as solvent, both electron-rich and electron-deficient boronic acids were successfully added to a range of cyclic N-acyliminium ions, typically with excellent diastereoselectivity with electron-deficient boron acids.
Platinum nanoparticle toxicity in freshwater algae and crustaceans: A physical or chemical effect?

General information
State: Published
Organisations: Department of Environmental Engineering, Environmental Chemistry, Department of Chemistry, NanoChemistry, Technical University of Denmark
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Number of pages: 2
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Preferential oxidation of CO in excess H₂ over CuO/CeO₂ catalysts: Performance as a function of the copper coverage and exposed face present in the CeO₂ support

CuO/CeO₂ catalysts where the support has different nanoparticle shapes exposing different lattice planes are examined for the preferential oxidation of CO in the presence of excess H₂ (CO-PROX reaction) in operando DRIFTS conditions. Even for catalysts with same surface concentration of Cu the selectivity for CO₂ formation is found close to 100% up to higher temperatures when the support is in form of nanocubes (exposing the less stable (001) lattice planes). DRIFTS data allow relating this to a higher stability of the Cu species forming the Cu⁺ carbonyls associated to the high activity and selectivity, so that they are fully reduced at higher temperature in agreement with TPR data. DFT calculations show that CuO nanoparticles interact more strongly (distorting more their structure) with the CeO₂ (001) surface than with the (111) surface, while XRD indicates that the formation of well developed CuO nanocrystals is more difficult on nanocube shaped CeO₂ than on other CeO₂ morphologies. Also EPR spectra show that the CuO entities nucleate on the ceria nanocubes differently. The higher stabilization of the oxidized state indicated by DFT, together with the mentioned structural distortion, may be then the reason for the improved selectivity.
Preparation and Characterization of Components for Intermediate Temperature Fuel Cells And Electrolyzers

The intermediate temperature region for fuel cells (200-400°C) is of interest as it may combine advantages from low and high temperature technologies. Increasing the temperature above what is used in polymer electrolyte membrane (PEM) fuel cells enhances the catalyst kinetics, and therefore it might become possible to use non-noble metal catalysts. On the other hand, the temperature is low enough for a wide range of materials to be used as construction materials. In this work a set-up was built and fuel cell hardware was made for demonstration of fuel cells for the intermediate temperature range. For the electrodes, carbon cloth and carbon paper were tested as gas diffusion layers with different catalytic compositions, and of the two, carbon paper with a platinum loading of 7 mg cm\(^{-2}\) had the better performance. However, carbon is unstable at the conditions in the fuel cell cathode and other materials must be sought for. It was attempted to use stainless steel (316L), this however corroded and therefore a protective tantalum coating was applied. The tantalum coatings were found to be corrosion resistant and furthermore provided extremely low interfacial contact resistances of only 1.3 m\(\Omega\) cm\(^2\). From a literature review it was found that the most promising results for this temperature range have been performed using cesium dihydrogen phosphate (CsH\(_2\)PO\(_4\)) electrolytes. CsH\(_2\)PO\(_4\) undergoes a phase transition at around 230°C, with a rise in conductivity from 8.5 \(\times\) 10\(^{-6}\) at 223°C to 1.8 \(\times\) 10\(^{-2}\) S cm\(^{-1}\) at 233°C this is called superprotonic. This electrolyte as well as other electrolytes for this temperature range, however, suffers from poor mechanical properties, and stable fuel cell performance had only been achieved by use of thick electrolytes. Furthermore to maintain high conductivity of the electrolyte, a high level of humidification was necessary. Composites with CsH\(_2\)PO\(_4\) were made to improve the properties of the electrolyte material. Composites in formation with mechanically strong materials including ZrO\(_2\), TiO\(_2\) and NdPO\(_4\)-0.5H\(_2\)O improved the densification of the electrolyte, which further resulted in improved stability of the fuel cell. Open circuit voltages (OCVs) using such fuel cells were found to be high, above 0.9 V, and stable up to 250°C. Composite formation with ZrO\(_2\) furthermore resulted in increased conductivity at higher temperatures probably due to the physical stabilization of the high conducting phase. At 250°C the cell was stable for more than 60 hours with a partial pressure of water of only 0.12 atm, and it was operational up to 275°C, where the fuel cell using pure CsH\(_2\)PO\(_4\) no longer performed. When CsH\(_2\)PO\(_4\) was used in composite with NdPO\(_4\)-0.5H\(_2\)O there were indications of a new phase formed, CsH\(_5\)(PO\(_4\))\(_2\), which has been reported to have high conductivity from 150°C. The mechanism behind an increase in conductivity for the CsH\(_2\)PO\(_4\)/NdPO\(_4\)-0.5H\(_2\)O ofvi several orders of magnitude was not fully clarified. Using an
29CsH2PO4/71NdPO4·H2O electrolyte enabled fuel cell performance measurements up to 285°C, where the highest performance was recorded. At this temperature current and power densities were found to be 117 mA cm−2 and 27.7 mW cm−2, respectively. Composite formation with melamine cyanurate resulted in increased conductivity in the entire temperature interval measured i.e. from 120°C to 260°C. A conductivity as high as 0.18 S cm−1 was measured for a 90CsH2PO4/10melamine cyanurate composite at 250°C. Good mechanical properties were furthermore observed for the composites. Within the research project a screening was made in order to search for new electrolytes. From this screening niobium and bismuth phosphates were found to have high conductivities (>10−2 S cm−1) with reasonable stability, and it was therefore attempted to fabricate electrochemical cells from these. The pure phosphates were however suffering from poor mechanical stability and therefore polybenzimidazole (PBI) was added. By adding high amounts of PBI stable OCVs were achieved, these remained stable for around 10 and 70 hours for niobium and bismuth phosphates, respectively. At high temperatures, however, the OCVs were found to drop, at 200°C the OCVs were below 0.9 V. Tungsten carbide was evaluated as a non-noble catalyst for the hydrogen evolution and oxidation reactions. Tungsten carbides were prepared in different ways in order to achieve higher surface areas compared to the very low surface area of the commercial carbide which was too low to be quantified. By preparing the carbide from WO3 (WC-mWO3) which had been prepared by use of a mesoporous silica template by carburization with methane at 900°C for 3 hours, a surface area of 6 m2 g−1 was measured. By introducing an extra synthesis step by first converting the WO3 into W2N which was then converted into WC (WC-mW2N) a higher surface area of 18 m2 g−1 was measured. The use of methane versus ethane as carburizing agents was investigated, by carburizing commercial WO3 with both agents under the same conditions. From carburization with methane no surface area could be quantified, while the carburization with ethane resulted in a carbide (WC-ethane) with a surface area of 12 m2 g−1. An additional tungsten carbide (WC-05-VN) with a BET area of 31 m2 g−1 was used for comparison. Hydrogen evolution activities for the carbides were measured in phosphoric acid at 185°C and -100 mV. It was found that apart from WC-mW2N, the activities were increasing with surface area, this deviation may be due to an amorphous carbon surface layer. Activities were found as 1.5, 2.07, 10.7 and 18.73 A g−1 for WC-mWO3, WC-mW2N, WC-ethane and WC-05-VN, respectively. The carbides were furthermore investigated as fuel cell anode catalysts. The best performances were achieved at the highest temperature measured i.e. 270°C where power densities of 2.7, 3.1, 7.4 and 8.2 mW cm−2 for WC-mW2N, WC-mWO3, WC-05-VN and WC-ethane, respectively, using CsH2PO4 electrolytes and WC loadings of 10 mg cm−2.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Proton conductors, Department of Chemistry
Authors: Jensen, A. H. (Intern), Bjerrum, N. J. (Intern), Christensen, E. (Intern), Li, Q. (Intern), Barner, J. H. V. (Intern)
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Probing interactions between B-glucan and bile salts at atomic detail by 1H-13C NMR assays
Polysaccharides are prospective hosts for the delivery and sequestration of bioactive guest molecules. Polysaccharides of dietary fiber, specifically cereal (1 → 3)(1 → 4)-β-glucans, play a role in lowering the blood plasma cholesterol level in humans. Direct host-guest interactions between β-glucans and conjugated bile salts are among the possible molecular mechanisms explaining the hypcholesterolemic effects of β-glucans. The present study shows that 1H-13C NMR assays on a time scale of minutes detect minute signal changes in both bile salts and β-glucans, thus indicating dynamic interactions between bile salts and β-glucans. Experiments are consistent with stronger interactions at pH 5.3 than at pH 6.5 in this in vitro assay. The changes in bile salt and β-glucan signals suggest a stabilization of bile salt micelles and concomitant conformational changes in β-glucans.

General information
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Organisations: Department of Chemistry, Organic Chemistry, Carlsberg Laboratory, University of Copenhagen
Authors: Mikkelsen, M. S. (Ekstern), Cornali, S. B. (Ekstern), Jensen, M. G. (Ekstern), Nilsson, L. M. (Ekstern), Beeren, S. (Intern), Meier, S. (Intern)
Pages: 11472-11478
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Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Agricultural and Food Chemistry
Probing Structural and Catalytic Characteristics of Galactose Oxidase Confined in Nanoscale Chemical Environments

Galactose oxidase (GAOX) is a special metalloenzyme in terms of its active site structure and catalytic mechanisms. This work reports a study where the enzyme confined in a nanoscale chemical environment provided by mesoporous silicas (MPS) is probed. Two types of MPS, i.e. SBA-15 and MCF, were synthesized and used to accommodate GAOX. SBA-15-ROD is rod-shaped particles with periodically ordered nanopores (9.5 nm), while MCF has a mesocellular foam-like structure with randomly distributed pores (23 nm) interconnected by smaller windows (8.8 nm). GAOX is non-covalently confined in SBA-15-ROD, while it is covalently immobilized in MCF. Relatively high loadings in the range of 50–60 mg g\(^{-1}\) are achieved. Electron spin resonance (ESR) spectroscopy is used to probe the active site structures of the enzyme. The similar ESR spectra observed for GAOX in the free and immobilized states support that the electronic structure, particularly the copper catalytic centre of confined GAOX is well retained. The catalytic activity of confined enzyme is high, although the catalytic kinetics is slowed down, mainly attributed to the diffusion limitation of substrate and product in the nanoscale channels. The apparent Michaelis constant (KM) of the enzyme is largely unchanged upon immobilization, while the turnover number (kcat) is slightly reduced. The overall catalytic efficiency, represented by the ratio of kcat/KM, is retained around 70% and 60% for SBA-15 and MCF immobilization, respectively. The thermal resistance is enhanced up to 60 °C, but with no further enhancement above 60 °C.

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Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, NanoChemistry
Authors: Ikemoto, H. (Intern), Mossin, S. (Intern), Ulstrup, J. (Intern), Chi, Q. (Intern)
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Web of Science (2016): Indexed yes
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BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.114 SNIP 0.965 CiteScore 3.87
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.117 SNIP 0.903 CiteScore 3.74
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Scopus rating (2012): SJR 0.863 SNIP 0.603 CiteScore 2.4
ISI indexed (2012): ISI indexed no
Web of Science (2012): Indexed yes
Original language: English
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Probing the structural details of xylan degradation by real-time NMR spectroscopy

The biodegradation of abundantly available cell wall polysaccharides has recently received much attention, not least because cell wall polysaccharides are substrates for the human gut microbiota and for environmentally sustainable processes of biomass conversion to value-added compounds. A major fraction of cereal cell wall polysaccharides consists of arabinoxylans. Arabinoxylan and its degradation products are therefore present in a variety of agro-industrial residues and products. Here, we undertook to track the structural details of wheat arabinoxylan degradation with high resolution NMR spectroscopy. More than 15 carbohydrate residues were distinguished in the substrate and more than 20 residues in partially degraded samples without any sample cleanup. The resolution of a plethora of structural motifs in situ permits the readout of persisting structures in degradation processes and in products. Reaction progress was visualized for the biodegradation of arabinoxylan by different crude microbial enzyme preparations. The direct observation of structural details in complex mixtures containing arabinoxylan fragments is significant, as such structural details reportedly modulate the health-promoting functions of arabinoxylan fragments.

General information

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Authors: Petersen, B. O. (Ekstern), Lok, F. (Ekstern), Meier, S. (Intern)
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Scopus rating (2016): CiteScore 5.15 SJR 1.404 SNIP 1.745
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.46 SNIP 1.842 CiteScore 4.86
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.584 SNIP 1.969 CiteScore 4.69
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.346 SNIP 1.967 CiteScore 4.39
ISI indexed (2013): ISI indexed yes
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Scopus rating (2012): SJR 1.409 SNIP 2.045 CiteScore 3.93
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Web of Science (2012): Indexed yes
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Scopus rating (2011): SJR 1.287 SNIP 1.991 CiteScore 4.08
ISI indexed (2011): ISI indexed yes
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BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.372 SNIP 1.808
Propargylamine-isothiocyanate reaction: efficient conjugation chemistry in aqueous media.
A coupling reaction between secondary propargyl amines and isothiocyanates in aqueous media is described. The reaction is high-yielding and affords cyclized products within 2-24 h. A functionalized ether lipid was synthesized in 8 steps, formulated as liposomes with POPC and conjugated to FITC under mild conditions using this method.

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry, Department of Micro- and Nanotechnology, Colloids and Biological Interfaces, Center for Nanomedicine and Theranostics, Technical University of Denmark
Authors: Viart, H. M. (Intern), Larsen, T. S. (Ekstern), Tassone, C. (Intern), Andresen, T. L. (Intern), Clausen, M. H. (Intern)
Pages: 7800-7802
Publication date: 2014
Main Research Area: Technical/natural sciences

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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
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Scopus rating (2014): SJR 2.701 SNIP 1.446 CiteScore 6.83
Web of Science (2014): Indexed yes
We consider a phase-locked two-pulse sequence applied to photofragmentation in the weak-field limit. The two pulses are not overlapping in time, i.e., the energy of the pulse-train is constant for all time delays. It is shown that the relative yield of excited Br* in the nonadiabatic process: I + Br*←IBr → I + Br, changes as a function of time delay when the two excited wave packets interfere. The underlying mechanisms are analyzed and the change in the branching ratio as a function of time delay is only a reflection of a changing frequency distribution of the pulse train; the branching ratio does not depend on the detailed pulse shape.

**General information**

State: Published
Organisations: Department of Chemistry, Physical and Biophysical Chemistry, Indian Institute of Science Education and Research
Quantification of leakage from large unilamellar lipid vesicles by fluorescence correlation spectroscopy

Fluorescence correlation spectroscopy (FCS) is a powerful experimental technique that in recent years has found numerous applications for studying biological phenomena. In this article, we scrutinize one of these applications, namely, FCS as a technique for studying leakage of fluorescent molecules from large unilamellar lipid vesicles. Specifically, we derive the mathematical framework required for using FCS to quantify leakage of fluorescent molecules from large unilamellar lipid vesicles, and we describe the appropriate methodology for successful completion of FCS experiments. By use of this methodology, we show that FCS can be used to accurately quantify leakage of fluorescent molecules from large unilamellar lipid vesicles, including leakage of fluorescent molecules of different sizes. To demonstrate the applicability of FCS, we have investigated the antimicrobial peptide mastoparan X. We show that mastoparan X forms transient transmembrane pores in POPC/POPG (3:1) vesicles, resulting in size-dependent leakage of molecules from the vesicles. We conclude the paper by discussing some of the advantages and limitations of FCS as compared to other existing methods to measure leakage from large unilamellar lipid vesicles.

General information
State: Published
Organisations: Department of Micro- and Nanotechnology, Colloids and Biological Interfaces, Center for Nanomedicine and Theranostics, Department of Chemistry, Physical and Biophysical Chemistry
Authors: Kristensen, K. (Intern), Henriksen, J. R. (Intern), Andresen, T. L. (Intern)
Pages: 2994-3002
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BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 1.511 SNIP 1.101 CiteScore 3.55
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.782 SNIP 1.142 CiteScore 3.8
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.869 SNIP 1.09 CiteScore 3.64
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.592 SNIP 0.975 CiteScore 3.45
ISI indexed (2013): ISI indexed yes
Quantitative monitoring of yeast fermentation using Raman spectroscopy

Compared to traditional IR methods, Raman spectroscopy has the advantage of only minimal interference from water when measuring aqueous samples, which makes this method potentially useful for in situ monitoring of important industrial bioprocesses. This study demonstrates real-time monitoring of a Saccharomyces cerevisiae fermentation process using a Raman spectroscopy instrument equipped with a robust sapphire ball probe. A method was developed to correct the Raman signal for the attenuation caused by light scattering cell particulate, hence enabling quantification of reaction components and possibly measurement of yeast cell concentrations. Extinction of Raman intensities to more than 50% during fermentation was normalized with approximated extinction expressions using Raman signal of water around 1,627 cm⁻¹ as an internal standard to correct for the effect of scattering. Complicated standard multi-variant chemometric techniques, such as PLS, were avoided in the quantification model, as an attempt to keep the monitoring method as simple as possible and still get satisfactory estimations. Instead, estimations were made with a two-step approach, where initial scattering correction of attenuated signals was followed by linear regression. In situ quantification measurements of the fermentation resulted in root mean square errors of prediction (RMSEP) of 2.357, 1.611, and 0.633 g/L for glucose, ethanol, and yeast concentrations, respectively.

General information
State: Published
Organisations: Department of Chemistry, Aalborg University
Quantum Mechanical Studies of DNA and LNA

Quantum mechanical (QM) methodology has been employed to study the structure activity relations of DNA and locked nucleic acid (LNA). The QM calculations provide the basis for construction of molecular structure and electrostatic surface potentials from molecular orbitals. The topologies of the electrostatic potentials were compared among model oligonucleotides, and it was observed that small structural modifications induce global changes in the molecular structure and surface potentials. Since ligand structure and electrostatic potential complementarity with a receptor is a determinant for the bonding pattern between molecules, minor chemical modifications may have profound changes in the interaction profiles of oligonucleotides, possibly leading to changes in pharmacological properties. The QM modeling data can be used to understand earlier observations of antisense oligonucleotide properties, that is, the observation that small structural changes in oligonucleotide composition may lead to dramatic shifts in phenotypes. These observations should be taken into account in future oligonucleotide drug discovery, and by focusing more on non RNA target interactions it should be possible to utilize the exhibited property diversity of oligonucleotides to produce improved antisense drugs.
This paper reports rational engineering of Trypanosoma rangeli sialidase to develop an effective enzyme for a potentially important type of reactivity: production of sialylated prebiotic glycans. The Trypanosoma cruzi trans-sialidase and the homologous T. rangeli sialidase has previously been used to investigate the structural requirements for trans-sialidase activity. We observed that the T. cruzi trans-sialidase has a seven-amino-acid motif (197–203) at the border of the substrate binding cleft. The motif differs substantially in chemical properties and substitution probability from the homologous sialidase, and we hypothesised that this motif is important for trans-sialidase activity. The 197–203 motif is strongly positively charged with a marked change in hydrogen bond donor capacity as compared to the sialidase. To investigate the role of this motif, we expressed and characterised a T. rangeli sialidase mutant, Tr13. Conditions for efficient trans-sialylation were determined, and Tr13’s acceptor specificity demonstrated promiscuity with respect to the acceptor molecule enabling sialylation of glycans containing terminal galactose and glucose and even monomers of glucose and fucose. Sialic acid is important in association with human milk oligosaccharides, and Tr13 was shown to sialylate a number of established and potential prebiotics. Initial evaluation of prebiotic potential using pure cultures demonstrated, albeit not selectively, growth of Bifidobacteria. Since the 197–203 motif stands out in the native trans-sialidase, is markedly different from the wild-type sialidase compared to previous mutants, and is shown here to confer efficient and broad trans-sialidase activity, we suggest that this motif can serve as a framework for future optimization of trans-sialylation towards prebiotic production.
Recognition of double-stranded DNA using energetically activated duplexes with interstrand zippers of 1-, 2- or 4-pyrenyl-functionalized O2'-alkylated RNA monomers

Despite advances with triplex-forming oligonucleotides, peptide nucleic acids, polyamides and more recently engineered proteins, there remains an urgent need for synthetic ligands that enable specific recognition of double-stranded (ds) DNA to accelerate studies aiming at detecting, regulating and modifying genes. Invaders, i.e., energetically activated DNA duplexes with interstrand zipper arrangements of intercalator-functionalized nucleotides, are emerging as an attractive approach toward this goal. Here, we characterize and compare Invaders based on 1-, 2- and 4-pyrenyl-functionalized O2'-alkylated uridine monomers X-Z by means of thermal denaturation experiments, optical spectroscopy, force-field simulations and recognition experiments using DNA hairpins as model targets. We demonstrate that Invaders with +1 interstrand zippers of X or Y monomers efficiently recognize mixed-sequence DNA hairpins with single nucleotide fidelity. Intercalator-mediated unwinding and activation of the double-stranded probe, coupled with extraordinary stabilization of probe target duplexes (Delta T-m/modification up to +14.0 degrees C), provides the driving force for dsDNA recognition.
contrast, Z-modified Invaders show much lower dsDNA recognition efficiency. Thus, even very conservative changes in the chemical makeup of the intercalator-functionalized nucleotides used to activate Invader duplexes, affects dsDNA-recognition efficiency of the probes, which highlights the importance of systematic structure property studies. The insight from this study will guide future design of Invaders for applications in molecular biology and nucleic acid diagnostics.

**General information**

State: Published
Organisations: Department of Chemistry, University of Idaho
Authors: Karmakar, S. (Ekstern), Madsen, A. S. (Intern), Guenther, D. C. (Ekstern), Gibbons, B. C. (Ekstern), Hrdlicka, P. J. (Ekstern)
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Main Research Area: Technical/natural sciences

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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.39 SJR 1.363 SNIP 0.803
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.41 SNIP 0.858 CiteScore 3.47
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.387 SNIP 0.903 CiteScore 3.5
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.481 SNIP 0.897 CiteScore 3.55
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.635 SNIP 0.934 CiteScore 3.47
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.737 SNIP 0.974 CiteScore 3.71
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.775 SNIP 0.951
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 1.831 SNIP 1.073
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 1.936 SNIP 1.042
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.843 SNIP 0.984
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.557 SNIP 0.957
Relationship between Beta-Lactoglobulin and Bovine Submaxillary Mucin: Structure and Tribology Studies

For food oral processing, any specific component in the food products and its structural changes in varying environment can give crucial influence on the sensory acceptance of the products. The objective of this research was to investigate the inter-action between beta-Lactoglobulin (BLG), the major whey protein, and bovine submaxillary mucin (BSM), a (model) major salivary component, when mixed (1:1) at different pHs (pH 3.0, 5.0 and 7.4) in order to broaden our understanding of food oral processing on the molecular level. High and low field Nuclear Magnetic Resonance (NMR), Dynamic Light Scattering (DLS) and Circular Dichroism (CD) techniques were employed to study the structural changes. A Mini-Traction Machine (MTM) was then employed to investigate the friction and lubrication properties of the proteins at a compliant interface, as a mimic of oral processing of dairy products.

Ring-opening of cyclic ethers with carbon–carbon bond formation by Grignard reagents

The ring-opening of cyclic ethers with concomitant C–C bond formation was studied with a number of Grignard reagents. The transformation was performed in a sealed vial by heating to ~160 °C in an aluminum block or at 180 °C in a microwave oven. Good yields of the product alcohols were obtained with allyl- and benzylmagnesium halides when the ether was tetrahydrofuran or 3,3-dimethyloxetane. Lower yields were obtained with substituted tetrahydrofurans while no ring-opening was observed with tetrahydropyran. Only highly reactive allyl and benzyl Grignard reagents participated in the transformation while no reaction occurred with other alkylmagnesium halides.

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry
Authors: Christensen, S. H. (Intern), Holm, T. (Intern), Madsen, R. (Intern)
Pages: 4942-4946
Publication date: 2014
Main Research Area: Technical/natural sciences
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 $O_2$ or $H_2O_2$ 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, physiosorption 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 carbontemplating 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
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**Selective synthesis of clinoatacamite Cu2(OH)3Cl and tenorite CuO nanoparticles by pH control**

Copper nanomaterials play a role as catalysts in sustainable energy technology and sensor devices. We present a one-pot synthesis for the selective preparation of phase-pure clinoatacamite (Cu₂(OH)₃Cl) and cupric oxide (CuO) nanoparticles by controlling the pH of the solution. The effect of pH on the phase of the product was systematically investigated utilizing 2-(N-morpholino)ethanesulfonic acid (MES) buffer. Here, the MES buffer was crucial for the synthesis. It not only allowed for selective synthesis by controlling pH but also guided the morphology of the CuO nanoparticles. In addition, it directed the growth of Cu₂(OH)₃Cl to provide pure clinoatacamite without the presence of related polymorphs. The products were characterized by transmission electron microscopy, infrared spectroscopy, ultraviolet–visible light spectroscopy, X-ray powder diffraction (XRD), scanning transmission X-ray microscopy and atomic force microscopy. Infrared spectroscopy was essential for characterization of closely related polymorphs of Cu₂(OH)₃Cl indistinguishable by XRD. A plausible mechanism has been proposed and discussed for the formation of the CuO and Cu₂(OH)₃Cl nanostructures.

**General information**

State: Published
Self-assembly of long chain fatty acids: Effect of a methyl branch

The morphology and molecular conformation of Langmuir-Blodgett deposited and floating monolayers of a selection of straight chain (eicosanoic acid, EA), iso (19-methyl eicosanoic acid, 19-MEA), and anteiso (18-methyl eicosanoic acid, 18-MEA) fatty acids have been investigated by Vibrational Sum Frequency Spectroscopy (VSFS), AFM imaging, and the Langmuir trough. While the straight chain fatty acid forms smooth, featureless monolayers, all the branched chain fatty acids display 10-50 nm sized domains (larger for 19-MEA than the 18-MEA) with a homogeneous size distribution. A model is suggested to explain the domain formation and size in terms of the branched fatty acid packing properties and the formation of hemispherical caps at the liquid-air interface. No difference between the chiral (S) form and the racemic mixture of the 18-MEA is observed with any of the utilized techniques. The aliphatic chains of the straight chain fatty acids appear to be oriented perpendicular to the sample surface, based on an orientational analysis of VSFS data and the odd/even effect. In addition, the selection of the subphase (neat water or CdCl2 containing water buffered to pH 6.0) used for the LB-deposition has a profound influence on the monolayer morphology, packing density, compressibility, and conformational order. Finally, the orientation of the 19-MEA dimethyl moiety is estimated, and a strategy for performing an orientational analysis to determine the complete molecular orientation of the aliphatic chains of 19-MEA and 18-MEA is outlined and discussed. This journal is © the Partner Organisations 2014.
Setting the stage for electron transfer: Molecular basis of ABTS-binding to four laccases from Trametes versicolor at variable pH and protein oxidation state

Laccases are multi-copper oxidases having exquisite oxidation power, high stability, and multiple industrial applications. Although Km varies ∼1000-fold across laccases, the molecular basis of substrate binding is poorly understood. Furthermore, laccase isoenzymes vary substantially in stability and activity for unknown reasons, and are thus useful probes of stability-function trade-offs relevant to protein engineering. We report here the first systematic comparison of ABTS-binding to different proteins, i.e. the four isoforms of Trametes versicolor, using a combination of sequence clustering, density functional theory calculations, homology modeling, and multiple induced-fit docking protocols at variable pH-dependent protonation states and T1-copper oxidation state. Clustering analysis provided a systematic overview of laccases across Trametes and revealed distinct isoenzyme classes (A–J) with the four T. versicolor isoforms belonging to separate classes. The T1 oxidation state had minor effect on ABTS binding, whereas the protonation state of Asp206 was important, consistent with site-directed mutagenesis studies. The absence of active poses for the δ-isoform agrees with its large Km, whereas the α-isoform with the smallest Km also had most active poses with protonated Asp206 corresponding to its pHopt∼2. Protonated Asp can bind to ABTS to form strong, active conformations partially explaining the low pHopt of fungal laccases toward ABTS. We identified several laccase properties optimal for ABTS binding. Notably, very high (R2∼0.99) correlation was observed between logKm (ABTS) and binding-pocket charge due to sites 157, 161, 269, 271, and 333, i.e. laccases optimal for ABTS turnover have positively charged anchor points in their pockets. Our work also demonstrates how activity-constraints can markedly improve docking to reduce inactive false positives.
Side Chain Hydrophobicity Modulates Therapeutic Activity and Membrane Selectivity of Antimicrobial Peptide Mastoparan-X

The discovery of new anti-infective compounds is stagnating and multi-resistant bacteria continue to emerge, threatening to end the "antibiotic era". Antimicrobial peptides (AMPs) and lipo-peptides such as daptomycin offer themselves as a new potential class of antibiotics; however, further optimization is needed if AMPs are to find broad use as antibiotics. In the present work, eight analogues of mastoparan-X (MPX) were investigated, having side chain modifications in position 1, 8 and 14 to modulate peptide hydrophobicity. The self-association properties of the peptides were characterized, and the peptide-membrane interactions in model membranes were compared with the bactericidal and haemolytic properties. Alanine substitution at position 1 and 14 resulted in higher target selectivity (red blood cells versus bacteria), but also decreased bactericidal potency. For these analogues, the gain in target selectivity correlated to biophysical parameters showing an increased effective charge and reduction in the partitioning coefficient for membrane insertion. Introduction of an unnatural amino acid, with an octyl side chain by amino acid substitution, at positions 1, 8 and 14 resulted in increased bactericidal potency at the expense of radically reduced membrane target selectivity. Overall, optimized membrane selectivity or bactericidal potency was achieved by changes in side chain hydrophobicity of MPX. However, enhanced potency was achieved at the expense of selectivity and vice versa in all cases.
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–amination–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)
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Simulations of Microbial-Enhanced Oil Recovery: Adsorption and Filtration

In the context of microbial-enhanced oil recovery (MEOR) with injection of surfactant-producing bacteria into the reservoir, different types of bacteria attachment and growth scenarios are studied using a 1D simulator. The irreversible bacteria attachment due to filtration similar to the deep bed filtration (DBF) is examined along with the commonly used reversible equilibrium adsorption (REA). The characteristics of the two models are highlighted. The options for bacteria growth are the uniform growth in both phases and growth of attached bacteria only. It is found that uniform growth scenario applied to filtration model provides formation of two oil banks during recovery. This feature is not reproduced by application of REA model or DBF with growth in attached phase. This makes it possible to select a right model based on the qualitative analysis of the experimental data. A criterion is introduced to study the process efficiency: the dimensionless time at which average recovery between pure water injection and maximum surfactant effect is reached. This characteristic recovery period (CRP) was studied as a function of the different MEOR parameters such as bacterial activity, filtration coefficients, and substrate injection concentrations. For both growth scenarios, there is a zone of optimal activity at which the CRP is minimal. Dependence of the CRP on substrate concentration for uniform growth scenario has an optimal zone. Therefore, growth rate and the substrate concentration should be above a certain threshold value and still not be too high to obtain the minimum CRP. On the other hand, no such zone was found if the bacteria could grow only in the attached phase. Dependencies on both the injected concentration and filtration coefficient are monotonous in this case.

General information
State: Published
Organisations: Center for Energy Resources Engineering, Department of Chemistry, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering
Authors: Nielsen, S. M. (Intern), Nesterov, I. (Intern), Shapiro, A. (Intern)
Pages: 227-259
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BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
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Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 2.16 SJR 0.767 SNIP 1.316
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.728 SNIP 1.317 CiteScore 1.94
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.932 SNIP 1.433 CiteScore 1.91
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.04 SNIP 1.433 CiteScore 2.03
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.942 SNIP 1.522 CiteScore 1.88
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.921 SNIP 1.337 CiteScore 1.81
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.615 SNIP 1.203
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Simultaneous Determination of Binding Constants for Multiple Carbohydrate Hosts in Complex Mixtures

We describe a simple method for the simultaneous determination of association constants for a guest binding to seven different hosts in a mixture of more than 20 different oligosaccharides. If the binding parameters are known for one component in the mixture, a single NMR titration suffices to determine binding constants for all other detectable and resolvable hosts. With the use of high-resolution 1H−13C HSQC experiments, complexes of amphiphiles with more than 10 different maltooligosaccharides can be resolved. Hereby, the binding capabilities of a set of structurally related hosts can be quantitatively studied to systematically explore noncovalent interactions without the need to isolate each host.

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry, Carlsberg Laboratory
Authors: Meier, S. (Intern), Beeren, S. (Intern)
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Volume: 136
Issue number: 32
ISSN (Print): 0002-7863
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 13.18 SJR 7.368 SNIP 2.584
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 6.826 SNIP 2.632 CiteScore 12.81
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 6.273 SNIP 2.578 CiteScore 11.92
Bacteria use small signaling molecules to communicate in a process termed “quorum sensing” (QS), which enables the coordination of survival strategies, such as production of virulence factors and biofilm formation. In Gram-negative bacteria, these signaling molecules are a series of N-acylated L-homoserine lactones. With the goal of identifying non-native compounds capable of modulating bacterial QS, a virtual library of N-dipeptido L-homoserine lactones was screened in silico with two different crystal structures of LasR. The 30 most promising hits were synthesized on HMBA-functionalized PEGA resin and released through an efficient acid-mediated cyclative release mechanism. Subsequent screening for modulation of QS in Pseudomonas aeruginosa and E. coli identified six moderately strong activators. A follow-up library designed from the preliminary derived structure–activity relationships was synthesized and evaluated for their ability to activate the QS system in this bacterium. This resulted in the identification of another six QS activators (two with low micromolar activity) thus illuminating structural features required for QS modulation.
Solid-phase synthesis of NH-1,2,3-triazoles using 4,4′-bismethoxybenzhydryl azide

Readily available 4,4′-bismethoxybenzhydryl azide was found to be a useful building block for the synthesis of NH-1,2,3-triazoles through copper(I)-catalyzed cycloaddition reactions with solid-supported terminal alkynes, followed by acid-mediated deprotection. Peptide-containing NH-1,2,3-triazoles were obtained in good yield and excellent purity (typically >95%).

General information
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Organisations: Department of Chemistry, Organic Chemistry
Authors: Cohrt, A. E. O. (Intern), Le Quement, S. T. (Intern), Nielsen, T. E. (Intern)
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Main Research Area: Technical/natural sciences

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BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.856 SNIP 0.461 CiteScore 1.84
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.875 SNIP 0.494 CiteScore 2
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.956 SNIP 0.574 CiteScore 2.09
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.017 SNIP 0.567 CiteScore 2.08
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.137 SNIP 0.623 CiteScore 2.1
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.288 SNIP 0.664 CiteScore 2.43
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.214 SNIP 0.63
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.261 SNIP 0.685
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Solid-phase synthesis of peptide thioureas and thiazole-containing macrocycles through ru-catalyzed ring-closing metathesis

N-Terminally modified α-thiourea peptides can selectively be synthesized on solid support under mild reaction conditions using N,N′-di-Boc-thiourea and Mukaiyama's reagent (2-chloro-1-methyl-pyridinium iodide). This N-terminal modification applies to the 20 proteinogenic amino acid residues on three commonly used resins for solid-phase synthesis. Complementary methods for the synthesis of α-guanidino peptides have also been developed. The thiourea products underwent quantitative reactions with α-halo ketones to form thiazoles in excellent purities and yields. When strategically installed between two alkene moieties, said thiazole core was conveniently embedded in peptide macrocycles via Ru-catalyzed ring-closing metathesis reactions. Various 15-17 membered macrocycles were easily accessible in all diastereomeric forms using this methodology. The developed "build/couple/pair" strategy is well suited for the generation of larger and stereochemically complete screening libraries of thiazole-containing peptide macrocycles.

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry
Authors: Cohrt, A. E. (Intern), Nielsen, T. E. (Intern)
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Volume: 16
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BFI (2018): BFI-level 1
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BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.16 SJR 1.019 SNIP 0.957
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.995 SNIP 0.953 CiteScore 3.13
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.008 SNIP 0.88 CiteScore 2.97
This thesis investigates different methods for improving reaction yields of enzyme-catalysed synthesis reactions. These methods include the use of non-conventional media such as ionic liquids (ILs) and organic solvents as main solvents or as co-solvents as well as the use of more classical reaction design methods, i.e. enzyme immobilization and the use of an enzymatic membrane reactor. Two different enzyme classes, namely feruloyl esterases (FAEs) and sialidases are employed.

Using sinapoylation of glycerol as a model reaction it was shown that both the IL anion nature and the FAE structure were important for FAE activity and stability in IL-buffer (15% v/v) systems. The quantum chemistry-based COSMO-RS method was applied for explaining the IL anion effect in terms of hydrogen bonding capacity. Furthermore, the usefulness of COSMO-RS and other thermodynamically based tools in solvent selection for FAE-catalysed acylation reactions was reviewed. FAE type A from Aspergillus niger and an FAE from a commercial preparation from Humicola insolens, Depol 740L, could not catalyse the esterification of arabinose or xylose with hydroxycinnamates in IL-buffer systems or in surfactantless microemulsion. However, both FAEs catalysed the feruloylation and/or sinapoylation of solvent cation C2OHIMIm+, thus underlining the broad acceptor specificity of FAEs and their potential for future solvent reactions.

An engineered sialidase from Trypanosoma rangeli, Tr6, catalyses trans-sialylation but the yield is hampered by substrate and product hydrolysis. The formation of 3'-sialyllactose from lactose and casein glycomacropeptide was used as a model reaction. Addition of 20-25% (v/v) t-butanol improved the trans-sialylation yield 1.4-fold and the synthesis/hydrolysis ratio 1.2-fold. Using ILs as co-solvents, the synthesis/hydrolysis ratio was also improved, but the trans-sialylation yield decreased, probably due to destabilization of Tr6 caused by the ILs. Returning to the conventional aqueous medium, immobilization of Tr6 on magnetic nanoparticles improved the synthesis/hydrolysis ratio 2.1-fold and increased the...
biocatalytic productivity of 2.5-fold. However, the recyclability of the immobilized enzyme was low. Reusing Tr6 seven times in a membrane reactor increased the trans-sialylation yield on the limiting substrate 1.3-fold, emphasizing the importance of the continuous product removal. Furthermore, the biocatalytic productivity was increased more than 9-fold as a result of the enzyme recovery.

In conclusion, where the use of non-conventional media is required for catalysis, e.g. in the thermodynamically controlled FAE-catalysed esterification, careful selection of both solvent system and the FAE itself is required to obtain adequate reaction yields. In contrast, for Tr6 the most promising results were obtained when keeping the reaction in aqueous medium and employing other reaction design methods such as continuous product removal and enzyme immobilization.

Steam reforming of ethanol over Ni-based catalysts: Effect of feed composition on catalyst stability

In this work the effects of steam-to-carbon ratio (S/C), and addition of H2 or O2 to the feed on the product yields and carbon deposition in the steam reforming (SR) of ethanol over Ni/MgAl2O4, Ni/Ce0.6Zr0.4O2, and Ni/CeO2 at 600 °C have been investigated. Increasing the S/C-ratio from 1.6 to 8.3 over Ni/MgAl2O4 increased conversion of ethanol as well as the yield of H2, while the carbon deposition and yield of hydrocarbons decreased. Oxygen addition at S/C-ratio of 6 over Ni/MgAl2O4, Ni/Ce0.6Zr0.4O2, and Ni/CeO2 increased conversion, decreased the yield of hydrocarbons, and led to a decrease in the carbon deposition. Carbon deposition was almost eliminated over Ni/MgAl2O4 and Ni/Ce0.6Zr0.4O2 at an O/C-ratio of roughly 0.8 or higher. The penalty of adding O2 was a decrease in the yield of H2 from 70% at O/C = 0 to 50% at O/C = 0.8–1. A 90 h test at O/C = 1.1, S/C = 6, and 600 °C over Ni/MgAl2O4 showed stable behavior and an average rate of carbon deposition of less than 7 μg C/gCat h. The results indicate that stable operation of ethanol SR is only possible under oxidative conditions.
Stereoselective Conversion of Glucosides into Xylosides

The demand for safe and healthy food is generally increasing and with it the interest in the functional ingredients in the consumed products. Among these ingredients are dietary fibers, which have attracted increased attention in research over the last decades, since the human health benefits from the consumption of fibers were scientifically demonstrated. Detailed studies of dietary fibers on a cellular level in plants benefits greatly from using the newest methods available in biotechnology such as specific monoclonal antibodies, which are a key-tool in protein-carbohydrate interactions, enzyme-linked immunosorbent assay (ELISA) and carbohydrate microarrays. To facilitate the development of monoclonal antibodies and characterization of their binding, it is necessary to obtain highly specific and pure oligosaccharides. However, methods for isolating acceptable quantities of required homogeneity from natural sources are difficult and time consuming, due to the heterogeneity and diversity of the plant cell wall polysaccharides. A alternative to isolation of oligosaccharides from the cell wall is chemical synthesis that makes it possible to obtain larger quantities of well-defined oligosaccharide structures in excellent purity.

This thesis describes the work on a new preparative synthesis method of D-xylose and D-xylobiose building blocks through carbohydrate interconversion of D-glucose and D-cellobiose. A range of methods for the transformation was investigated and the method of dehydrogenative decarbonylation was preferred because of its novelty and versatility. As
proof of concept, the building blocks were applied to the synthesis of oligoxylans. Furthermore, the method proved to be an alternative route for selective equatorial deuterium labeling of D-xylose by stereo retention, whereas radical methods mainly afforded axial deuteriation.

The work at University of Leeds during the external stay is described. It consisted of the utilization of monoclonal antibodies, ELISA and epitope detecting chromatography for the investigation of polysaccharides found in Arabidopsis thaliana root mucilage and mutants hereof.

**General information**
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Organisations: Department of Chemistry, Organic Chemistry
Authors: Pedersen, M. J. (Intern), Clausen, M. H. (Intern)
Number of pages: 158
Publication date: 2014

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Original language: English
Main Research Area: Technical/natural sciences
Publication: Research › Ph.D. thesis – Annual report year: 2015

**Strontium Localization in Bone Tissue Studied by X-Ray Absorption Spectroscopy**
Strontium has recently been introduced as a pharmacological agent for the treatment and prevention of osteoporosis. We determined the localization of strontium incorporated into bone matrix from dogs treated with Sr malonate by X-ray absorption spectroscopy. A new approach for analyzing the X-ray absorption spectra resulted in a compositional model and allowed the relative distribution of strontium in the different bone components to be estimated. Approximately 35–45 % of the strontium present is incorporated into calcium hydroxyapatite (CaHA) by substitution of some of the calcium ions occupying highly ordered sites, and at least 30 % is located at less ordered sites where only the first solvation shell is resolved, suggesting that strontium is surrounded by only oxygen atoms similar to Sr2+ in solution. Strontium was furthermore shown to be absorbed in collagen in which it obtains a higher structural order than when present in serum but less order than when it is incorporated into CaHA. The total amount of strontium in the samples was determined by inductively coupled plasma mass spectrometry, and the amount of Sr was found to increase with increasing dose levels and treatment periods, whereas the relative distribution of strontium among the different components appears to be independent of treatment period and dose level.

**General information**
State: Published
Organisations: Department of Chemistry, X-ray Crystallography
Authors: Frankær, C. G. (Intern), Raffalt, A. C. (Intern), Ståhl, K. (Intern)
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Web of Science (2018): Indexed yes
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Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 1.207 SNIP 1.08 CiteScore 3.05
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.184 SNIP 1.182 CiteScore 3.13
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.164 SNIP 1.122 CiteScore 2.99
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.168 SNIP 1.162 CiteScore 3
ISI indexed (2013): ISI indexed yes
Structural and functional characterization of protein complexes in the blood coagulation cascade

In this dissertation, components of coagulation factor (F)X-activating (tenase; fXase) complexes are studied using computational biophysics and the molecular dynamics (MD) method. The main focus is on structure-function relationships of the two central tenase complexes with respect to activation processes, complex formation, and platelet membrane association. Both the intrinsic and the extrinsic tenase complex consists of a trypsin-like serine protease and auxiliary domains complexed with the appropriate cofactor; FIXa with FVIIIa and FVIIa with tissue factor (TF), respectively. Topics covered will include the structural and dynamical changes upon proteolytic activation and TF-induced allosteric activation of FVIIa. In addition, FVIIa variants with the 170-loop grafted from trypsin will be looked into and, in particular, the mechanisms that enable these variants to have increased activity without TF are explained. Furthermore, the inter-domain linker connecting the two epidermal growth factor-like domains of FVIIa will be discussed with respect to consequences for its ability to form a productive complex with tissue factor. Finally, membrane binding of FVIIIa as mediated by the tandem C2-like domains is described using a highly mobile membrane-mimetic model.
Structural determination of Streptococcus pneumoniae repeat units in serotype 41A and 41F capsular polysaccharides to probe gene functions in the corresponding capsular biosynthetic loci

We report the repeating unit structures of the native capsular polysaccharides of S. pneumoniae serotypes 41A and 41F. Structural determinations yielded six carbohydrate units in the doubly branched repeating unit to give the following structure for serotype 41A: The structure determinations were motivated (1) by an ambition to help close the remaining gaps in S. pneumoniae capsular polysaccharide structures, and (2) by the attempt to derive functional annotations of carbohydrate active enzymes in the biosynthesis of bacterial polysaccharides from the determined structures. A new activity present in 41F but not 41A is identified as an acetyltransferase acting on the rhamnopyranosyl sidechain E. The genes encoding the formation of the six glycosidic bonds in serogroup 41 were determined from the capsular polysaccharide structures of serotype 41A, 41F and genetically related serotypes, in conjunction with corresponding genomic information and computational homology searches. In combination with complementary information, NMR spectroscopy considerably simplifies the functional annotation of carbohydrate active enzymes in the biosynthesis of bacterial polysaccharides.
Substrate binding activates the designed triple mutant of the colicin E7 metallonuclease.
The nuclease domain of colicin E7 (NColE7) cleaves DNA nonspecifically. The active center is a Zn(2+)-containing HNH motif at the C-terminus. The N-terminal loop is essential for the catalytic activity providing opportunity for allosteric modulation of the enzyme. To identify the key residues responsible for the structural integrity of NColE7, a virtual alanine scan was performed on a semiempirical quantum chemical level within the 25 residue long N-terminal sequence (446-470). Based on the calculations the T454A/K458A/W464A-NColE7 triple mutant (TKW) was expressed and purified. According to the agarose gel electrophoresis experiments and linear dichroism spectra the catalytic activity of the TKW mutant decreased in comparison with wild-type NColE7. The distorted structure and weakened Zn(2+) binding may account for this as revealed by circular dichroism spectra, mass spectrometry, fluorescence-based thermal analysis and isothermal microcalorimetric titrations. Remarkably, the substrate induced the folding of the mutant protein.

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State: Published
Organisations: Department of Chemistry, Metalloprotein Chemistry and Engineering, MTA-SZTE Bioinorganic Chemistry Research Group, University of Szeged, Academy of Sciences of the Czech Republic, University of Copenhagen, University of Tsukuba
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Main Research Area: Technical/natural sciences

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Volume: 19
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ISSN (Print): 0949-8257
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Web of Science (2018): Indexed yes
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Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.857 SNIP 0.761 CiteScore 2.4
Sucrose acetate isobutyrate based nanogels as liquid fiducial tissue markers with potential use in image guided radiotherapy

General information
State: Published
Organisations: Department of Micro- and Nanotechnology, Center for Nanomedicine and Theranostics, Department of Chemistry, Organic Chemistry, Colloids and Biological Interfaces, Technical University of Denmark, Copenhagen University Hospital
Authors: Bruun, L. M. (Intern), Schaarup-Jensen, H. (Intern), Jelck, R. I. (Intern), Hansen, A. E. (Intern), Christiansen, A. N. (Ekstern), Clausen, M. H. (Intern), Kjær, A. (Ekstern), Scherman, P. J. B. (Ekstern), Andresen, T. L. (Intern)
Number of pages: 1
Publication date: 2014
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Main Research Area: Technical/natural sciences
Electronic versions:
Abstract_Poster_Liposome_Research_Days_and_TOKS_2014.pdf
Sucrose acetate isobutyrate-based nanogels as liquid fiducial tissue markers with potential use in image guided radiotherapy

The poster presents the development of a liquid fiducial tissue marker based on sucrose acetate isobutyrate (SAIB) and uniform, coated gold nanoparticles (AuNPs). The PNIPAM-coated AuNP-SAIB gel provided high CT contrast and high in vivo stability and was assessed to be a suitable tissue marker for image guided radiotherapy (IGRT).

Superior DeNOx activity of V2O5-WO3/TiO2 catalysts prepared by deposition–precipitation method

V2O5-WO3/TiO2 catalysts were prepared by incipient wetness impregnation and deposition–precipitation (DP) methods. The catalysts were characterized by N2 physisorption, X-ray powder diffraction, Fourier transform infra red spectroscopy, electron paramagnetic resonance spectroscopy, transmission electron microscopy, H2-temperature programmed reduction and NH3-temperature programmed desorption. The catalysts exhibited only crystalline TiO2 phases with the active metal and promoter in highly dispersed or amorphous state. The 3 wt% V2O5–10 wt% WO3/TiO2 catalyst prepared by DP using ammonium carbamate as a precipitating agent was found to be the most active and selective to N2. The superior activity of the catalyst can be ascribed to the altered acidic and redox properties of vanadium. The catalysts did not show increased potassium resistance with the change in preparation method or with increasing vanadium concentration. Furthermore, potassium-poisoned catalysts showed above stoichiometric loss of surface acidity. Thus, these modified formulations are suggested to be used in coal/natural gas-fired power plants where there is a demand for high selective catalytic reduction activity and selectivity to N22.
Supported Rh-phosphine complex catalysts for continuous gas-phase decarbonylation of aldehydes.

Heterogeneous silica supported rhodium-phosphine complex catalysts are employed for the first time in the catalytic decarbonylation of aldehydes in continuous gas-phase. The reaction protocol is exemplified for the decarbonylation of p-tolualdehyde to toluene and further extended to other aromatic and aliphatic aldehydes achieving excellent results in terms of both conversion and selectivity.

**General information**

State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, NanoChemistry
Authors: Malcho, P. (Intern), Garcia-Suarez, E. J. (Intern), Mentzel, U. V. (Intern), Engelbrekt, C. (Intern), Riisager, A. (Intern)
Pages: 17230-17235
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Main Research Area: Technical/natural sciences

**Publication information**

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- BFI (2017): BFI-level 2
- Web of Science (2017): Indexed Yes
- BFI (2016): BFI-level 2
- Scopus rating (2016): CiteScore 3.85 SJR 1.243 SNIP 0.931
- Web of Science (2016): Indexed yes
- BFI (2015): BFI-level 2
- Scopus rating (2015): SJR 1.351 SNIP 1.026 CiteScore 4.1
- Web of Science (2015): Indexed yes
- BFI (2014): BFI-level 2
- Scopus rating (2014): SJR 1.413 SNIP 1.085 CiteScore 4.06
- Web of Science (2014): Indexed yes
- BFI (2013): BFI-level 1
- Scopus rating (2013): SJR 1.436 SNIP 1.083 CiteScore 4.07
- ISI indexed (2013): ISI indexed yes
- Web of Science (2013): Indexed yes
- BFI (2012): BFI-level 1
- Scopus rating (2012): SJR 1.554 SNIP 1.001 CiteScore 3.79
- ISI indexed (2012): ISI indexed yes
- Web of Science (2012): Indexed yes
- BFI (2011): BFI-level 1
- Scopus rating (2011): SJR 1.505 SNIP 1.013 CiteScore 3.68
- ISI indexed (2011): ISI indexed yes
- BFI (2010): BFI-level 1
Responsive biomaterial hydrogels attract significant attention due to their biocompatibility and degradability. In order to make chitosan based gels, we first graft one layer of chitosan to silica, and then build a chitosan/poly(acrylic acid) multilayer using the layer-by-layer approach. After cross-linking the chitosan present in the polyelectrolyte multilayer, poly(acrylic acid) is partly removed by exposing the multilayer structure to a concentrated carbonate buffer solution at a high pH, leaving a surface-grafted cross-linked gel. Chemical cross-linking enhances the gel stability against detachment and decomposition. The chemical reaction between gluteraldehyde, the cross-linking agent, and chitosan was followed in situ using total internal reflection Raman (TIRR) spectroscopy, which provided a molecular insight into the complex reaction mechanism, as well as the means to quantify the cross-linking density. The amount of poly(acrylic acid) trapped inside the surface grafted films was found to decrease with decreasing cross-linking density, as confirmed in situ using TIRR, and ex situ by Fourier transform infrared (FTIR) measurements on dried films. The responsiveness of the chitosan-based gels with respect to pH changes was probed by quartz crystal microbalance with dissipation (QCM-D) and TIRR. Highly cross-linked gels show a small and fully reversible behavior when the solution pH is switched between pH 2.7 and 5.7. In contrast, low cross-linked gels are more responsive to pH changes, but the response is fully reversible only after the first exposure to the acidic solution, once an internal restructuring of the gel has taken place. Two distinct pKa's for both chitosan and poly(acrylic acid), were determined for the cross-linked structure using TIRR. They are associated with populations of chargeable groups displaying either a bulk like dissociation behavior or forming ionic complexes inside the hydrogel film. © 2014 American Chemical Society.
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Surface grafted chitosan gels. Part I. Molecular insight into the formation of chitosan and poly(acrylic acid) multilayers

Composite polyelectrolyte multilayers of chitosan and low molecular weight poly(acrylic acid) (PAA) have been assembled by sequential adsorption as a first step toward building a surface anchored chitosan gel. Silane chemistry was used to graft the first chitosan layer to prevent film detachment and decomposition. The assembly process is characterized by nonlinear growth behavior, with different adsorption kinetics for chitosan and PAA. In situ analysis of the multilayer by means of surface sensitive total internal reflection Raman (TIRR) spectroscopy, combined with target factor analysis of the spectra, provided information regarding composition, including water content, and ionization state of weak acidic and basic groups present in the thin composite film. Low molecular weight PAA, mainly in its protonated form, diffuses into and out of the composite film during adsorption and rinsing steps. The higher molecular weight chitosan shows a similar behavior, although to a much lower extent. Our data demonstrate that the charged monomeric units of chitosan are mainly compensated by carboxylate ions from PAA. Furthermore, the morphology and mechanical properties of the multilayers were investigated in situ using atomic force microscopy operating in PeakForce tapping mode. The multilayer consists of islands that grow in lateral dimension and height during the build-up process, leading to close to exponentially increasing roughness with deposition number. Both diffusion in and out of at least one of the two components (PAA) and the island-like morphology contribute to the nonlinear growth of chitosan/PAA multilayers. © 2014 American Chemical Society.

General information
State: Published
Organisations: Department of Chemistry, KTH - Royal Institute of Technology
Authors: Liu, C. (Ekstern), Thormann, E. (Intern), Claesson, P. M. (Ekstern), Tyrode, E. (Ekstern)
Pages: 8866-8877
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Main Research Area: Technical/natural sciences

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Web of Science (2017): Indexed Yes
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Scopus rating (2016): CiteScore 3.99 SJR 1.55 SNIP 1.188
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.686 SNIP 1.308 CiteScore 4.33
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.816 SNIP 1.391 CiteScore 4.59
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.895 SNIP 1.356 CiteScore 4.55
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Synchrotron X-ray diffraction study of thermal decomposition of expanded austenite

General information
State: Published
Organisations: Department of Mechanical Engineering, Materials and Surface Engineering, Department of Chemistry, X-ray Crystallography
Authors: Brink, B. (Intern), Ståhl, K. (Intern), Christiansen, T. L. (Intern), Somers, M. A. J. (Intern)
Number of pages: 1
Publication date: 2014
Main Research Area: Technical/natural sciences
Expanded austenite, In-situ, Thermal decomposition
Electronic versions:
Abstract_EPDIC14.pdf
Source: PublicationPreSubmission
Source-ID: 116663951
Synergy between experimental and theoretical methods in the exploration of homogeneous transition metal catalysis

In this Perspective, we will focus on the use of both experimental and theoretical methods in the exploration of reaction mechanisms in homogeneous transition metal catalysis. We briefly introduce the use of Hammett studies and kinetic isotope effects (KIE). Both of these techniques can be complemented by computational chemistry – in particular in cases where interpretation of the experimental results is not straightforward. The good correspondence between experiment and theory is only possible due to recent advances within the applied theoretical framework. We therefore also highlight the innovations made in the last decades with emphasis on dispersion-corrected DFT and solvation models. The current state-of-the-art is highlighted using examples from the literature with particular focus on the synergy between experiment and theory.

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry
Authors: Lupp, D. (Intern), Christensen, N. J. (Intern), Fristrup, P. (Intern)
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BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 3.85 SJR 1.243 SNIP 0.931
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 1.351 SNIP 1.026 CiteScore 4.1
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 1.413 SNIP 1.085 CiteScore 4.06
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.436 SNIP 1.083 CiteScore 4.07
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.554 SNIP 1.001 CiteScore 3.79
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.505 SNIP 1.013 CiteScore 3.68
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.399 SNIP 0.875
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 0.928 SNIP 0.783
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Synthesis and Application of Plant Cell Wall Oligogalactans

The plant cell walls represent almost 50% of the biomass found in plants and are therefore one of the main targets for biotechnological research. Major motivators are their potential as a renewable energy source for transport fuels, as functional foods, and as a source of raw materials to generate chemical building blocks for industrial processes. To achieve a sustainable development it is necessary to optimize plant production and utilization. This will require a better understanding of the cell wall structure and function at the molecular level.

The cell wall is composed by an intricate network of polysaccharides and proteins that changes during the different developmental stages of the cell. This makes it very challenging to address the function of individual components in living cells. Alternatively, structurally defined oligosaccharides can be used as models for the more complex polysaccharide components in order to investigate a range of properties such as cell wall biosynthesis and protein-carbohydrate interactions. The oligosaccharides can be obtained by chemical or enzymatic degradation of the cell wall. However, although extensive studies have been conducted only a limited range of structures is available and the obtained oligosaccharides require extensive purification. Chemical synthesis, on the other hand, is capable of producing structurally diverse oligosaccharides of excellent purity and in higher quantities.

This thesis presents the chemical synthesis of fragments of galactans and arabinogalactans that are prominent side chains of the pectic polysaccharide rhamnogalacturonan I (RG-I) and the main component of arabinogalactan protein (AGP). In the galactan series, 16 linear or branched β-(1→4)-linked D-galactosides of four to eight residues were prepared by a convergent block strategy. Using a disaccharide donor the number of glycosylations were reduced significantly and late stage regioselective deprotection made it possible to introduce various branches. By the same general strategy, seven linear or branched β-(1→3)-linked- and three linear β-(1→6)-linked D-galactosides were prepared as part of the arabinogalactans series. The fragments were applied in the characterization of a glycosyl transferase, a hydrolase and to study the important cancer biomarker galectin-3. The work done during an external stay at University of Oxford is also presented. This concerns isolation and modification of the carbohydrate-based antibiotic, Tunicamycin. A simple and effective method has been developed for chemo-enzymatic synthesis of the partially protected core tunicaminyl lactol. Furthermore, synthesis of several novel muramic acid donors and attempts to glycosylate the tunicaminy lactol are discussed.
Synthesis and Characterization of Divalent Manganese, Iron, and Cobalt Complexes in Tripodal Phenolate/N-Heterocyclic Carbene Ligand Environments

Two novel tripodal ligands, (BIMPNMes,Ad,Me)− and (MIMPNMes,Ad,Me)2−, combining two types of donor atoms, namely, NHC and phenolate donors, were synthesized to complete the series of N-anchored ligands, ranging from chelating species with tris(carbene) to tris(phenolate) chelating arms. The complete ligand series offers a convenient way of tuning the electronic and steric environment around the metal center, thus, allowing for control of the complex’s reactivity. This series of divalent complexes of Mn, Fe, and Co was synthesized and characterized by 1H NMR, IR, and UV/vis spectroscopy as well as by single-crystal X-ray diffraction studies. Variable-temperature SQUID magnetization measurements in the range from 2 to 300 K confirmed high-spin ground states for all divalent complexes and revealed a trend of increasing zero-field splitting |D| from Mn(II), to Fe(II), to Co(II) complexes. Zero-field 57Fe Mössbauer spectroscopy of the Fe(II) complexes 3, 4, 8, and 11 shows isomer shifts δ that increase gradually as carbenes are substituted for phenolates in the series of ligands. From the single-crystal structure determinations of the complexes, the different steric demand of the ligands is evident. Particularly, the molecular structure of 1 in which a pyridine molecule is situated next to the Mn–Cl bond and those of azide complexes 2, 4, and 6 demonstrate the flexibility of these mixed-ligand derivatives, which, in contrast to the corresponding symmetrical TIMENR ligands, allow for side access of, e.g., organic substrates, to the reactive metal center.
Synthesis and crystal structures of 2-methyl-4-aryl-5-oxo-5H-indeno [1,2-b] pyridine carboxylate derivatives

Background: Hantzsch 1,4-dihydropyridines (Hantzsch1,4-DHP) have been extensively utilized as the analogs of nicotinamide adenine dinucleotide (NADH) coenzyme to study the mechanism and various redox processes. During the redox processes 1,4-DHP systems undergo transformation into the corresponding pyridine derivatives through oxidation. Consequently, the interest in this aromatization reaction, investigation of a wide range of 1, 4-DHPs continues to attract the attention of researchers. Herein, we report the preparation of pyridine derivatives and the crystal structures determined by X-ray crystallographic methods.

Results: The crystal structures and conformational studies of two organic compounds, namely ethyl 2-methyl-4-phenyl-5-oxo-5H-indeno [1,2-b] pyridine-3-carboxylate (I) and ethyl 2-methyl-4-(4 chlorophenyl)-5-oxo-5H-indeno [1,2-b] pyridine-3-carboxylate (II) are reported. The terminal ethyl group of the compound I is disordered over two positions with the refined occupancies of 0.645 & 0.355 and C8 one dimensional zig-zag chain running along 101 direction through C-H..O type of intermolecular interactions. In the compound II, the substitution of Cl atom in the phenyl ring alters the configuration of carboxylate group with respect to the pyridine indane ring.

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General information
State: Published
Organisations: Department of Chemistry, Physical and Biophysical Chemistry, University of Madras, Mother Teresa Women’s University, Roskilde University
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Synthesis and Evaluation of Desmethyl Azumamide Analogs

Histone deacetylases (HDACs) are a group of epigenetic modulators, which catalyze the removal of e-Nacetylated lysine residues. Histones are the most studied targets, however, the acetylated state of a variety of other proteins are also modified by HDACs. Aberrant epigenetic processes have been associated with various types of cancer and HDACs have therefore been a target in the development of anticancer drugs. So far, two HDAC inhibitors have been approved by the food and drug administration (FDA) and several compounds are in clinical trials.

Macrocyclic HDAC inhibitors are interesting compounds, as they can interact with a variety of amino acids on the surface near the binding site; these interactions may be used to obtain selectivity for specific HDAC isozymes. The azumamides are potent HDAC inhibitors and since they possess a relatively weak zinc-binding group (ZBG), the activity must arise from interactions with the large cap group. The natural compounds have been used as an inspiration to synthesize new HDAC inhibitors.

A small structure activity relationship (SAR) study was conducted in collaboration with Jesper S. Villadsen. Aromatic substituents in the cyclic peptide were explored, while the primary modifications were done to the b-amino acid. Removal of the methyl group in the 2-position and changes to the unsaturation in the side at the 3-position, afforded six compounds. These were tested against HDAC enzymes from class I, IIb, and IV.

Minor changes in activity were observed among the azumamide analogs; however, removal of the methyl group had a significant impact relative to the natural products. To understand this effect, the NMR structure was solved with the assistance from Casper Hoeck and Charlotte H. Gotfredsen and docked conformations were obtained from Niels J. Christensen and Peter Fristrup. Compared to the natural compounds, the 3Dstructure of the scaffold in the azumamide
analogs were similar. Although a conclusion was not found, the preliminary docking results indicated favorable lipophilic interaction with the methyl group in the azumamides.

Largazole is another macrocyclic natural product with HDAC inhibitory activity. The compound has a thioester functionality in the side chain, which is hydrolyzed before interaction with the enzymes. In the attempt to mimic the prodrug nature of largazole, compounds containing a thiol group were designed, as it was hypothesized that acylation with different lipids could generate compounds with improved cell penetrating properties. A desmethylated azumamide analog containing a thiol side chain was synthesized and tested against HDAC3. A low activity was observed, which was explained by the unfavorable linker length.

In the work performed at CalTech, five 2-a-phenylpyrroloindolines were synthesized; utilizing an NCS mediated cyclization as the key step. Chris Marotta and Christina McCleary Daeffler tested their effect against a variety of ligand-gated ion-channels. Among these, one compound proved to be an agonist for the GABAA receptor.

**General information**
State: Published
Organisations: Department of Chemistry
Authors: Maolanon, A. (Intern), Olsen, C. A. (Intern)
Number of pages: 154
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**Synthesis of 4-Halogenated 3-Fluoro-6-methoxyquinolines: Key Building Blocks for the Synthesis of Antibiotics**
A practical and scalable 4-step route is presented for the synthesis of 4-bromo-3-fluoro-6-methoxyquinoline and 3-fluoro-4-iodo-6-methoxyquinoline from readily available 2,4-dichloro-3-fluoroquinoline with an overall yield of 81-85%. Halogenated quinoline building blocks have found much use in antimicrobial drug discovery, and the method reported here would be useful for the synthesis of these compounds. © Georg Thieme Verlag.

**General information**
State: Published
Organisations: Department of Chemistry, Organic Chemistry, University of Copenhagen
Authors: Flagstad, T. (Intern), Petersen, M. T. (Intern), Hinnerfeldt, D. M. (Intern), Givskov, M. C. (Ekstern), Nielsen, T. E. (Intern)
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Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 1.046 SNIP 0.575 CiteScore 2.34
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.088 SNIP 0.669 CiteScore 2.39
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.079 SNIP 0.694 CiteScore 2.43
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.126 SNIP 0.675 CiteScore 2.37
ISI indexed (2013): ISI indexed yes
Massive efforts in molecular library synthesis have strived for the development of synthesis methodology which systematically delivers natural product-like compounds of high spatial complexity. Herein, we present a conceptually simple approach that builds on the power of solid-phase peptide synthesis to assemble precursor peptides (oligomers) designed to undergo oxidative cascade reactions. By harnessing the structural side-chain diversity and inherent stereochemical features offered by readily available amino acids (monomers), a proof-of-concept collection of 54 skeletally and stereochemically diverse compounds was generated, and selected compounds were elaborated into isoform-selective metalloprotease inhibitors.
Synthesis of a Natural Product-Like Compound Collection through Oxidative Cleavage and Cyclization of Linear Peptides.

Massive efforts in molecular library synthesis have strived for the development of synthesis methodology which systematically delivers natural product-like compounds of high spatial complexity. Herein, we present a conceptually simple approach that builds on the power of solid-phase peptide synthesis to assemble precursor peptides (oligomers) designed to undergo oxidative cascade reactions. By harnessing the structural side-chain diversity and inherent stereochemical features offered by readily available amino acids (monomers), a proof-of-concept collection of 54 skeletally and stereochemically diverse compounds was generated, and selected compounds were elaborated into isoform-selective metalloprotease inhibitors.

**General information**

State: Published
Organisations: Department of Chemistry, Organic Chemistry
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- Web of Science (2016): Indexed yes
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- BFI (2014): BFI-level 1
- Web of Science (2014): Indexed yes
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- 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
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Original language: English
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**Synthesis of heterocycles through transition-metal-catalyzed isomerization reactions**

Metal-catalyzed isomerization of N- and O-allylic systems is emerging as an effective method to form synthetically useful iminium and oxocarbenium intermediates. In the presence of tethered nucleophiles, several recent examples illuminate this approach as a powerful strategy for the synthesis of structurally complex and diverse heterocycles. In this Concept article, we attempt to cover this area of research through a selection of recent versatile examples. A sea of opportunities! Transition-metal-catalyzed isomerization of N- and O-allylic compounds provides a mild, selective and synthetically versatile method to form iminium and oxocarbenium ions. Given the number of reactions involving these highly electrophilic intermediates, this concept provides a sea of opportunities for heterocycle synthesis, (see scheme; Nu=nucleophile). © 2014 WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim.

**General information**
Synthesis of Oxacyclic Scaffolds via Dual Ruthenium Hydride/Brønsted Acid-Catalyzed Isomerization/Cyclization of Allylic Ethers

A ruthenium hydride/Brønsted acid-catalyzed tandem sequence is reported for the synthesis of 1,3,4,9-tetrahydropyrano[3,4-b]indoles (THPIs) and related oxacyclic scaffolds. The process was designed on the premise that readily available allylic ethers would undergo sequential isomerization, first to enol ethers (Ru catalysis), then to oxocarbenium ions (Brønsted acid catalysis) amenable to endo cyclization with tethered nucleophiles. This methodology provides not only an attractive alternative to the traditional oxa-Pictet–Spengler reaction for the synthesis of THPIs, but also convenient access to THPI congeners and other important oxacycles such as acetals.

General information
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ISSN (Print): 0947-6539
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BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 5.03 SJR 2.247 SNIP 1.046
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 2.416 SNIP 1.184 CiteScore 4.99
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.487 SNIP 1.219 CiteScore 5.51
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.604 SNIP 1.239 CiteScore 5.68
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 2.884 SNIP 1.294 CiteScore 5.55
ISI indexed (2012): ISI indexed yes
Synthesis of substituted gamma-lactams through petasis-type addition of boronic acids to N-acyliminium ions

Substituted \( \gamma \)-lactams are important heterocyclic motifs found in various biologically active compounds and marketed drugs, such as glimepiride, doxapram, and levetiracetam. Among available methods for the synthesis of substituted \( \gamma \)-lactams, the addition of nucleophiles to N-acyliminium ions remains the most widely utilized approach. Even though hydroxylactams are important precursors of cyclic N-acyliminium ions, few approaches for their synthesis have been reported so far. By implementing a reductive cyclization reaction, linear L-malic acid derivatives were rapidly converted into cyclic N-acyliminium ions. Under the optimized conditions, entailing the use of HFIP as solvent, both electron-rich and electron-deficient boronic acids were successfully added to a range of cyclic N-acyliminium ions, thereby obtaining a collection of pharmaceutically relevant substituted \( \gamma \)-lactams.
The antimalarial drug quinine interferes with serotonin biosynthesis and action

The major antimalarial drug quinine perturbs uptake of the essential amino acid tryptophan, and patients with low plasma tryptophan are predisposed to adverse quinine reactions; symptoms of which are similar to indications of tryptophan depletion. As tryptophan is a precursor of the neurotransmitter serotonin (5-HT), here we test the hypothesis that quinine disrupts serotonin function. Quinine inhibited serotonin-induced proliferation of yeast as well as human (SHSY5Y) cells. One possible cause of this effect is through inhibition of 5-HT receptor activation by quinine, as we observed here. Furthermore, cells exhibited marked decreases in serotonin production during incubation with quinine. By assaying activity and kinetics of the rate-limiting enzyme for serotonin biosynthesis, tryptophan hydroxylase (TPH2), we showed that quinine competitively inhibits TPH2 in the presence of the substrate tryptophan. The study shows that quinine disrupts both serotonin biosynthesis and function, giving important new insight to the action of quinine on mammalian cells.
The Chemistry of Griseofulvin

Specific synthetic routes are presented in schemes to illustrate the chemistry, and the analogs are presented in a table format to give an accessible overview of the structures. Several patents have been published regarding the properties of griseofulvin and its derivatives including synthesis, formulation, and their medicinal and agricultural applications. The antifungal mode-of-action of griseofulvin has been the subject of considerable research efforts and some debate over the years, a discussion that is still ongoing. Griseofulvin was one of the first antifungal natural products found in filamentous fungi. During the years, this polyketide has been found to be produced by several Ascomycetes including both closely and distantly related species.

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry, Center for Nanomedicine and Theranostics, Department of Systems Biology
Authors: Petersen, A. B. (Intern), Rønnest, M. H. (Intern), Larsen, T. O. (Intern), Clausen, M. H. (Intern)
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Main Research Area: Technical/natural sciences

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Volume: 114
Issue number: 24
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 42.79 SJR 19.282 SNIP 10.369
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 18.373 SNIP 11.51 CiteScore 45.92
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 18.369 SNIP 11.47 CiteScore 44.56
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 22.176 SNIP 12.915 CiteScore 49.12
ISI indexed (2013): ISI indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 20.511 SNIP 11.43 CiteScore 39.08
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 19.538 SNIP 11.534 CiteScore 39.19
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 18.393 SNIP 11.114
BFI (2009): BFI-level 2
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 16.038 SNIP 8.682
Web of Science (2008): Indexed yes
The effect of hydrogen bonding on torsional dynamics: A combined far-infrared jet and matrix isolation study of methanol dimer.

The effect of strong intermolecular hydrogen bonding on torsional degrees of freedom is investigated by far-infrared absorption spectroscopy for different methanol dimer isotopologues isolated in supersonic jet expansions or embedded in inert neon matrices at low temperatures. For the vacuum-isolated and Ne-embedded methanol dimer, the hydrogen bond OH librational mode of the donor subunit is finally observed at ∼560 cm⁻¹, blue-shifted by more than 300 cm⁻¹ relative to the OH torsional fundamental of the free methanol monomer. The OH torsional mode of the acceptor embedded in neon is observed at ∼286 cm⁻¹. The experimental findings are held against harmonic predictions from local coupled-cluster methods with single and double excitations and a perturbative treatment of triple excitations [LCCSD(T)] and anharmonic VPT2 corrections at canonical MP2 and density functional theory (DFT) levels in order to quantify the contribution of vibrational anharmonicity for this important class of intermolecular hydrogen bond vibrational motion.

General information
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Organisations: Department of Chemistry, X-ray Crystallography, Georg-August-Universität Göttingen, Lund University
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 2.13 SJR 1.073 SNIP 0.755
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 0.953 SNIP 0.767 CiteScore 1.98
The Effect of Various Zinc Binding Groups on Inhibition of Histone Deacetylases 1–11

Histone deacetylases (HDACs) have the ability to cleave the acetyl groups of ε-N-acetylated lysine residues in a variety of proteins. Given that human cells contain thousands of different acetylated lysine residues, HDACS may regulate a wide variety of processes including some implicated in conditions such as cancer and neurodegenerative disorders. Herein we report the synthesis and in vitro biochemical profiling of a series of compounds, including known inhibitors as well as novel
chemotypes, that incorporate putative new zinc binding domains. By evaluating the compound collection against all 11 recombinant human HDACs, we found that the trifluoromethyl ketone functionality provides potent inhibition of all four subclasses of the Zn2+-dependent HDACs. Potent inhibition was observed with two different scaffolds, demonstrating the efficiency of the trifluoromethyl ketone moiety as a zinc binding motif. Interestingly, we also identified silanediol as a zinc binding group with potential for future development of non-hydroxamate class I and class IIb HDAC inhibitors.

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry, Department of Chemistry
Authors: Madsen, A. S. (Intern), Kristensen, H. M. E. (Intern), Lanz, G. (Intern), Olsen, C. A. (Intern)
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Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
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Scopus rating (2016): SJR 1.13 SNIP 0.906 CiteScore 3.11
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.148 SNIP 0.905 CiteScore 3
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.11 SNIP 0.907 CiteScore 2.83
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.142 SNIP 0.845 CiteScore 2.93
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.125 SNIP 0.814 CiteScore 2.87
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.263 SNIP 0.928 CiteScore 3.24
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.264 SNIP 0.923
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.188 SNIP 0.89
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.272 SNIP 0.905
Scopus rating (2007): SJR 0.991 SNIP 1.127
Web of Science (2007): Indexed yes
Scopus rating (2006): SNIP 0.9
Scopus rating (2005): SNIP 0.85
Scopus rating (2004): SNIP 0.847
Scopus rating (2003): SNIP 0.911
Scopus rating (2002): SNIP 0.83
Scopus rating (2001): SNIP 0.628
The influence of selection for protein stability on dN/dS estimations.

Understanding the relative contributions of various evolutionary processes—purifying selection, neutral drift, and adaptation—is fundamental to evolutionary biology. A common metric to distinguish these processes is the ratio of nonsynonymous to synonymous substitutions (i.e., dN/dS) interpreted from the neutral theory as a null model. However, from biophysical considerations, mutations have non-negligible effects on the biophysical properties of proteins such as folding stability. In this work, we investigated how stability affects the rate of protein evolution in phylogenetic trees by using simulations that combine explicit protein sequences with associated stability changes. We first simulated myoglobin evolution in phylogenetic trees with a biophysically realistic approach that accounts for 3D structural information and estimates of changes in stability upon mutation. We then compared evolutionary rates inferred directly from simulation to those estimated using maximum-likelihood (ML) methods. We found that the dN/dS estimated by ML methods (ωML) is highly predictive of the per gene dN/dS inferred from the simulated phylogenetic trees. This agreement is strong in the regime of high stability where protein evolution is neutral. At low folding stabilities and under mutation-selection balance, we observe deviations from neutrality (per gene dN/dS > 1 and dN/dS <1). We showed that although per gene dN/dS is robust to these deviations, ML tests for positive selection detect statistically significant per site dN/dS > 1. Altogether, we show how protein biophysics affects the dN/dS estimations and its subsequent interpretation. These results are important for improving the current approaches for detecting positive selection.
The Non-Ergodic Nature of Internal Conversion

The absorption of light by molecules can induce ultrafast dynamics and coupling of electronic and nuclear vibrational motion. The ultrafast nature in many cases rests on the importance of several potential energy surfaces in guiding the nuclear motion—a concept of central importance in many aspects of chemical reaction dynamics. This Minireview focuses on the non-ergodic nature of internal conversion, that is, on the concept that the nuclear dynamics only sample a reduced phase space, potentially resulting in localization of the dynamics in real space. A series of results that highlight the nonstatistical nature of the excited-state deactivation process is presented. The examples are categorized into four groups. 1) Localization of the energy in one degree of freedom in S2|S1 transitions, in which the transition is either determined by the time spent in the S2|S1 coupling region or by the time it takes to reach it. 2) Localization of energy into a single reactive mode, which is dictated by the internal conversion process. 3) Initiation of the internal conversion by activation of a single complex motion, which then specifically couples to a reactive mode. 4) Nonstatistical internal conversion as a tool to accomplish biomolecular stability. Herein, the discussion on nonstatistical internal conversion in DNA as a mechanism to eliminate Electronic excitation energy is extended to include molecules with an SS bond as a model of the disulfide bridge in peptides. All of these examples are summed up in Kasha’s rule. For systems with multiple degrees of freedom it will be possible to locate an appropriate motion somewhere in phase space that will take the wavepacket to the coupling region and facilitate an ultrafast transition to S1. Once at S1, the momentum of the wavepacket is lost and the only options left are the statistical processes of reaction or light emission.

General information
State: Published
Organisations: Department of Chemistry, Maersk Oil Research and Technology Centre, University of Copenhagen
Authors: Sølling, T. I. (Ekstern), Kuhlman, T. S. (Intern), Stephansen, A. B. (Ekstern), Klein, L. B. (Ekstern), Møller, K. B. (Intern)
Pages: 249 – 259
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Main Research Area: Technical/natural sciences

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Web of Science (2014): Indexed yes
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BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.763 SNIP 0.955 CiteScore 3.24
ISI indexed (2012): ISI indexed yes
The retro Grignard addition reaction revisited: the reversible addition of benzyl reagents to ketones
The Grignard addition reaction is known to be a reversible process with allylic reagents, but so far the reversibility has not been demonstrated with other alkylmagnesium halides. By using crossover experiments it has been established that the benzyl addition reaction is also a reversible transformation. The retro benzyl reaction was shown by the addition of benzylmagnesium chloride to di-tert-butyl ketone followed by exchange of both the benzyl and the ketone moiety with another substrate. Similar experiments were performed with phenylmagnesium bromide and tert-butylmagnesium chloride, but in these two cases the Grignard addition reaction did not show any sign of a reverse transformation.

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry
Authors: Christensen, S. H. (Intern), Holm, T. (Intern), Madsen, R. (Intern)
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Nitrogen-expanded austenite, _N, with high and low nitrogen contents was produced from AISI 316 grade stainless steel powder by gaseous nitriding in ammonia/hydrogen gas mixtures. In situ synchrotron X-ray diffraction was applied to investigate the thermal expansion and thermal stability of expanded austenite in the temperature range 385–920 K. Evaluation of the diffractograms of the sample with a high nitrogen content, corresponding to an occupancy of the interstitial lattice of 56%, with Rietveld refinement yielded a best convergence after including the stacking fault probability.
as a fitting parameter. The stacking fault density is constant for temperatures up to 680 K, whereafter it decreases to nil. Surprisingly, a transition phase with composition M4N (M = Fe, Cr, Ni, Mo) appears for temperatures above 770 K. The linear coefficient of thermal expansion depends on the nitrogen content and is lowest for the sample with a high level of nitrogen.
Theoretical modeling of complex systems

Offshore reservoirs represent one of the major growth areas of the oil and gas industry, and environmental safety is one of the biggest challenges for the offshore exploration and production. The oil accidents in the Gulf of Mexico in 1979 and 2010 were two of the biggest disasters in history. Contrary to earlier theories, the oil is not only present on the surface, but also in great volumes both in the water column and on the seafloor, which indicates that we do not know enough about how oil behaves in water and interacts with it. Sonar detection is one of the most important and necessary technologies to reduce the environmental effects of offshore oil exploration. It could be used (1) to detect oil and gas leaks around the subsea well head enabling faster responses, especially in deep water and/or ice covered areas; (2) to detect and map the oil in the seawater column during cleanup process after an oil spill. Engineering thermodynamics could be applied in the state-of-the-art sonar products through advanced artificial technology, if the speed of sound, solubility and density of oil-seawater systems could be satisfactorily modelled. The addition of methanol or glycols into unprocessed well streams during subsea pipelines is necessary to inhibit gas hydrate formation, and the offshore reservoirs often mean complicated temperature and pressure conditions. Accurate description of the phase behavior and thermophysical properties of complex systems containing petroleum fluids and polar compounds are extremely important from viewpoints of the economical operation and environmental safety. The classical thermodynamic models used by the oil industry are semi-empirical and not suitable for mixtures containing water and other polar chemicals. The complex nature of water, its anomalous properties due to hydrogen bonding and the hydrophobic interactions with hydrocarbons (oils), are not described well by such simple models. The perturbation theory based models have an explicit term to account for the hydrogen bonding, and these models are also believed to have better performance for derivative properties, e.g. speed of sound, and for density under extreme conditions. This PhD thesis studies the capabilities and limitations of the Perturbed-Chain Statistical Association Fluid Theory (PC-SAFT) equation of state. It consists of three parts. In the first part, the PC-SAFT EOS is successfully applied to model the phase behaviour of water, chemical and hydrocarbon (oil) containing systems with newly developed pure component parameters for water and chemical and characterization procedures for petroleum fluids. The performance of the PCSAFT EOS on liquid-liquid equilibria of water with hydrocarbons has been under debate for some vii years. An interactive step-wise procedure is proposed to fit the model parameters for small associating fluids by taking the liquid-liquid equilibrium data into account. It is still far away from a simple task to apply PC-SAFT in routine PVT simulations and phase behaviour of petroleum fluids. It has been extensively studied on how to develop general petroleum fluid characterization approaches for PC-SAFT. The performance of the newly developed parameters and characterization procedures for the description of the phase equilibria of well- and ill-defined binary and ternary systems containing water, chemicals and/or hydrocarbons (oils) is quite satisfactory, if compared to the models available in literature. The modeling of petroleum fluid-water-MEG systems provides further information to develop simpler and more robust characterization approaches. In the second part, the speed of sound data and their correlations of various systems are reviewed. Two approaches are proposed to improve the speed of sound description within the PC-SAFT framework by putting speed of sound data into the parameter estimation and/or the universal constant regression. The first approach works only for short associating fluids, while the second approach significantly improves the speed of sound description for various systems both qualitatively and quantitatively. The possibility of simultaneous modeling of phase behavior and speed of sound, including the effects of parameter estimation approaches for 1-alcohol containing systems, are also investigated. In the third part, the fundamentals of PC-SAFT are investigated based on the universal constant regression. The PC-SAFT EOS has been criticized for some numerical pitfalls during the recent years. A new variant of universal constants has been developed, which has avoided the numerical pitfalls of having more than three volume roots in the real application range. It has been shown that it is possible to directly use the original PC-SAFT parameters with the new universal constants for the systems considered in this thesis. Finally, the salt effects on the solubility of hydrocarbons, the speed of sound, and the static permittivity of aqueous solutions are briefly discussed. It is still an open question how to estimate the model parameters for associating fluids with pure component properties only. The possibility of using the static permittivity data in the parameter estimation is discussed by adopting a newly developed theory of static permittivity and association theory based EOS.
Three-Dimensional Reduced Graphene Oxide Network on Copper Foam as High-performance Supercapacitor Electrodes

Electrochemically generated copper foam (Cuf) could serve as an effective template for fabrication of three-dimensional (3D) reduced graphene oxide (rGO) networks. Here we present a facile approach to preparation of 3D rGO networks supported by Cuf as binder-free and current collector-integrated supercapacitor electrodes (3DrGO@Cuf) [1]. The method involves a two-step procedure, self-assembly of graphene oxide (GO) nanosheets on Cuf and electrochemical reduction of GO into rGO. We have systematically characterized as-synthesized materials using AFM, SEM and XRD to reveal their morphological and structural features. Electrochemical functional tests show that such electrodes are capable of delivering a specific capacitance as high as 623 F g\(^{-1}\) at a current density of 1 A g\(^{-1}\). The observed high specific capacitance is most likely attributed to the unique porous structure consisting of highly connected nano scale pores and high-density capacitive sites. 3DrGO@Cuf electrodes also exhibit considerably high stability over successive charge-discharge switching. For example, over 98% specific capacitance is retained after 2000 cycles. To the best of our knowledge, we may have achieved the highest specific capacitance with 3DrGO@Cuf electrodes among reported pure 3D graphene materials to date (i.e. 3D graphene materials without doping additional capacitive species) [2, 3].

THz absorption spectrum of the CO\(_2\)-H\(_2\)O complex: Observation and assignment of intermolecular van der Waals vibrations

Terahertz absorption spectra have been recorded for the weakly bound CO\(_2\)-H\(_2\)O complex embedded in cryogenic neon matrices at 2.8 K. The three high-frequency van der Waals vibrational transitions associated with out-of-plane wagging, in-plane rocking, and torsional motion of the isotopic H\(_2\)O subunit have been assigned and provide crucial observables for benchmark theoretical descriptions of this system's flat intermolecular potential energy surface. A (semi)-empirical value for the zero-point energy of 273 ± 15 cm\(^{-1}\) from the class of intermolecular van der Waals vibrations is proposed and the combination with high-level quantum chemical calculations provides a value of 726 ± 15 cm\(^{-1}\) for the dissociation energy D\(_0\).
Time-resolved photoelectron spectroscopy and ab initio multiple spawning studies of hexamethylcyclopentadiene

Time-resolved photoelectron spectroscopy and ab initio multiple spawning were applied to the ultrafast non-adiabatic dynamics of hexamethylcyclopentadiene. The high level of agreement between experiment and theory associates wavepacket motion with a distinct degree of freedom.

General information

State: Published
Organisations: Department of Chemistry, Karlsruhe Institute of Technology KIT, Stockholm University, Stanford University, University of Ottawa
Authors: Wolf, T. J. A. (Ekstern), Kuhlman, T. S. (Intern), Schalk, O. (Ekstern), Martínez, T. J. (Ekstern), Møller, K. B. (Intern), Stolow, A. (Ekstern), Unterreiner, A. (Ekstern)
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Tomato Cutin Deficient 1 (CD1) and putative orthologs comprise an ancient family of cutin synthase-like (CUS) proteins that are conserved among land plants

The aerial epidermis of all land plants is covered with a hydrophobic cuticle that provides essential protection from desiccation, and so its evolution is believed to have been prerequisite for terrestrial colonization. A major structural component of apparently all plant cuticles is cutin, a polyester of hydroxy fatty acids; however, despite its ubiquity, the details of cutin polymeric structure and the mechanisms of its formation and remodeling are not well understood. We recently reported that cutin polymerization in tomato (Solanum lycopersicum) fruit occurs via transesterification of hydroxyacylglycerol precursors, catalyzed by the GDSL-motif lipase/hydrolase family protein (GDSL) Cutin Deficient 1 (CD1). Here, we present additional biochemical characterization of CD1 and putative orthologs from Arabidopsis thaliana and the moss Physcomitrella patens, which represent a distinct clade of cutin synthases within the large GDSL superfamily. We demonstrate that members of this ancient and conserved family of cutin synthase-like (CUS) proteins act as polyester synthesases with negligible hydrolytic activity. Moreover, solution-state NMR analysis indicates that CD1 catalyzes the formation of primarily linear cutin oligomeric products in vitro. These results reveal a conserved mechanism of cutin polyester synthesis in land plants, and suggest that elaborations of the linear polymer, such as branching or cross-linking, may require additional, as yet unknown, factors.
Microorganisms are an attractive source of new natural products with antimicrobial properties, and the marine environment constitutes a prolific resource of bioactive microorganisms. During a global research expedition (Galathea III), two depsipeptides, solonamide A and solonamide B, were isolated from the marine bacterium Photobacterium halotolerance and were found to inhibit virulence gene expression in the serious human pathogen, Staphylococcus aureus. They act by interfering with the agr quorum sensing system and show resemblance to the endogenous S. aureus quorum sensing peptide, autoinducing peptide I (AIP-I). To enable more comprehensive studies, we embarked on the chemical synthesis of solonamides A and B. The key synthetic steps were formation of the (R)-β-hydroxy-fatty-acids by stereo-selective aldol reactions and a cyclative macrolactamization, which proceeded under highly dilute conditions. Thus, the first total syntheses of the solonamides corroborated the originally assigned structures, and by changing the stereochemistry of the auxiliary in the aldol steps we gained access to the natural products as well as their β3-epimers.
Towards accurate structural characterization of metal centres in protein crystals: the structures of Ni and Cu T6 bovine insulin derivatives

Using synchrotron radiation (SR), the crystal structures of T6 bovine insulin complexed with Ni2+ and Cu2+ were solved to 1.50 and 1.45 Å resolution, respectively. The level of detail around the metal centres in these structures was highly limited, and the coordination of water in Cu site II of the copper insulin derivative was deteriorated as a consequence of radiation damage. To provide more detail, X-ray absorption spectroscopy (XAS) was used to improve the information level about metal coordination in each derivative. The nickel derivative contains hexacoordinated Ni2+ with trigonal symmetry, whereas the copper derivative contains tetragonally distorted hexacoordinated Cu2+ as a result of the Jahn-Teller effect, with a significantly longer coordination distance for one of the three water molecules in the coordination sphere. That the copper centre is of type II was further confirmed by electron paramagnetic resonance (EPR). The coordination distances were refined from EXAFS with standard deviations within 0.01 Å. The insulin derivative containing Cu2+ is sensitive towards photoreduction when exposed to SR. During the reduction of Cu2+ to Cu+, the coordination geometry of copper changes towards lower coordination numbers. Primary damage, i.e. photoreduction, was followed directly by XANES as a function of radiation dose, while secondary damage in the form of structural changes around the Cu atoms after exposure to different radiation doses was studied by crystallography using a laboratory diffractometer. Protection against photoreduction and subsequent radiation damage was carried out by solid embedment of Cu insulin in a saccharose matrix. At 100 K the photoreduction was suppressed by ~15%, and it was suppressed by a further 30% on cooling the samples to 20 K.
Tracking developmentally regulated post-synthetic processing of homogalacturonan and chitin using reciprocal oligosaccharide probes.

Polysaccharides are major components of extracellular matrices and are often extensively modified post-synthetically to suit local requirements and developmental programmes. However, our current understanding of the spatiotemporal dynamics and functional significance of these modifications is limited by a lack of suitable molecular tools. Here, we report the development of a novel non-immunological approach for producing highly selective reciprocal oligosaccharide-based probes for chitosan (the product of chitin deacetylation) and for demethylesterified homogalacturonan. Specific reciprocal binding is mediated by the unique stereochemical arrangement of oppositely charged amino and carboxy groups. Conjugation of oligosaccharides to fluorophores or gold nanoparticles enables direct and rapid imaging of homogalacturonan and chitosan with unprecedented precision in diverse plant, fungal and animal systems. We demonstrated their potential for providing new biological insights by using them to study homogalacturonan processing during Arabidopsis thaliana root cap development and by analyzing sites of chitosan deposition in fungal cell walls and arthropod exoskeletons.
**Transient Changes in Molecular Geometries and How to Model Them**

Light-induced chemical processes are accompanied by molecular motion on the femtosecond time scale. Uncovering this dynamical motion is central to understanding the chemical reaction on a fundamental level. This thesis focuses on the aspects of excess excitation energy dissipation via dynamic changes in molecular structure, vibrations and solvation. In this thesis, we employ our recently developed Quantum-Mechanical Direct Dynamics method to do simulations of transition metal complexes in solution, to uncover their energy dissipation channels, and how they are affected by the solvent. The simulations has also served as benchmarks on this newly developed implementation. First, we establish that the chosen model provides a trustworthy description of the systems; since transition metals are heavier than purely organic systems, we test a range of approximations to relativistic quantum mechanic descriptions, to ascertain the accuracy of the quantum model in the Direct Dynamics simulations. We then test - and improve - the framework for calculating the experimental X-ray Diffuse Scattering Difference signal from (any kind of) Molecular Dynamics (MD) simulations. Comparisons of purely classical MD simulations to literature Direct Dynamics simulations delineate the boundaries for the force-field approximation: Classical MD provides a solvent shell response sufficient for experimental fits, but fails to model specific solvent shell changes, such as intercalation. The first Direct Dynamics project of this work focuses on a bi-metallic Ir complex, where the excited state bond formation results in a large Ir-Ir contraction with oscillatory behaviour. Forty simulated excited state trajectories of 3.5 ps each compare well with experimental results, and uncover a new vibrational mode. We observe how the wide distribution of ground state geometries is responsible for decoherence, and that the solvent cage actually facilitates coherent motion, by blocking the newly discovered vibrational mode. We furthermore observe a non-specific, rotational solvent response to the excitation. The second Direct Dynamics project studies the effect of solvation on a bi-centred Ru-Co complex, and we observe how the intercalation solvation response which was lost in the study using only force-fields, is recovered in the Direc Dynamics description.

**General information**

State: Published
Organisations: Center for Atomic-scale Materials Design, Department of Chemistry, Physical and Biophysical Chemistry
Authors: Dohn, A. O. (Intern), Møller, K. B. (Intern), Henriksen, N. E. (Intern)
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Source-ID: 105598969
Publication: Research - Ph.D. thesis – Annual report year: 2015

**Triazatriangulene as binding group for molecular electronics**

The triazatriangulene (TATA) ring system was investigated as a binding group for tunnel junctions of molecular wires on gold surfaces. Self-assembled monolayers (SAMs) of TATA platforms with three different lengths of phenylene wires were fabricated, and their electrical conductance was recorded by both conducting probe-atomic force microscopy (CP-AFM) and scanning tunneling microscopy (STM). Similar measurements were performed for phenylene SAMs with thiol anchoring groups as references. It was found that, despite the presence of a sp3 hybridized carbon atom in the conduction path, the TATA platform displays a contact resistance only slightly larger than the thiols. This surprising finding has not been reported before and was analyzed by theoretical computations of the transmission functions of the TATA anchored molecular wires. The relatively low contact resistance of the TATA platform along with its high stability and directionality make this binding group very attractive for molecular electronic measurements and devices. (Figure Presented).

**General information**

State: Published
Organisations: Department of Micro- and Nanotechnology, Self-Organized Nanoporous Materials, Department of Chemistry, NanoChemistry, University of Copenhagen, Chinese Academy of Sciences
Authors: Wei, Z. (Ekstern), Wang, X. (Ekstern), Borges, A. (Ekstern), Santella, M. (Ekstern), Li, T. (Intern), Sørensen, J. K. (Ekstern), Vanin, M. (Ekstern), Hu, W. (Ekstern), Liu, Y. (Ekstern), Ulstrup, J. (Intern), Solomon, G. C. (Ekstern), Chi, Q. (Intern), Bjørnholm, T. (Ekstern), Nergaard, K. (Ekstern), Laursen, B. W. (Ekstern)
Pages: 14868-14876
Publication date: 2014
Main Research Area: Technical/natural sciences

**Publication information**
Unexpected Secoiridoid Glucosides from Manulea corymbosa

From an extract of Manulea corymbosa were isolated four known secoiridoid glucosides (1–4), 10 new monoterpenoid esters of secologanol, namely, manuleosides A–I (5–11, 13, and 14) and dimethyl rhodanthoside A (12), and four new phenylpropanoid esters of carbocyclic iridoid glucosides, manucorymbosides I–IV (15–18). Also, the caffeoyl phenylethanoid glycoside verbascoside was isolated. The presence of secoiridoids apparently derived from loganic acid in the family Scrophulariaceae is unprecedented and greatly unexpected.
Unmixing the NMR spectra of similar species – vive la différence

Diffusion-ordered spectroscopy (DOSY) is one of the most powerful methods for intact mixture analysis by NMR. However, the separation of overlapped spectra by current DOSY methods typically requires a minimum of 30% difference in diffusion coefficient. Here we present a new algorithm (OUTSCORE) that can improve the situation by almost an order of magnitude, allowing the unmixing of severely overlapped species of similar size, by combining least squares fitting with cross-talk minimisation, maximising spectral difference.

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry, University of Manchester
Authors: Colbourne, A. A. (Ekstern), Meier, S. (Intern), Morris, G. A. (Ekstern), Nielsson, M. (Ekstern)
Pages: 10510--10512
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Scopus rating (2016): CiteScore 6.06 SJR 2.506 SNIP 1.159
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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
X-ray powder diffraction: a powerful analysis tool for industrial protein production

General information
State: Published
Authors: Frankær, C. G. (Intern), Thymark, M. (Ekstern), Ståhl, K. (Intern), Moroz, O. V. (Ekstern), Wilson, K. S. (Ekstern), Harris, P. (Intern)
Number of pages: 1
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Event: Abstract from 23rd Congress and General Assembly of the International Union of Crystallography, Montréal, Canada.
Zeolite-catalyzed isomerization of tetrose in aqueous medium

The isomerization of erythrose (ERO) was studied in water over commercially available large-pore zeolites such as, e.g., H-Y, H-USY and H-beta. Among the employed zeolites, H-USY(6) was found to efficiently isomerize the sugar yielding 45% erythrulose (ERU), 42% ERO and 3% of the epimer threose (THO) (corresponding to the equilibrium mixture), i.e., total tetrose yield 90%, after reaction for 5-7 h at 120 °C. Changing the solvent from water to methanol decreased the yield of ERU markedly to 18%, and gave only a total yield of tetroses of 27% which is significantly lower than obtained in water. Hence, the results demonstrate water to be a preferred solvent compared to lower alcohols for zeolite-catalyzed tetrose isomerization, which is opposite to what previously have been found for analogous pentose and hexose isomerization. A reuse study revealed further that H-USY(6) could be applied in at least five reaction runs with essentially unchanged activity and without significant aluminium leaching from the catalyst. The use of benign reaction conditions and an industrially pertinent solid catalyst in combination with water establishes a new, green tetrose isomerization protocol.
Zeolitic Materials

General information
State: Published
Organisations: Department of Chemistry, X-ray Crystallography
Authors: Ståhl, K. (Intern)
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Main Research Area: Technical/natural sciences

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Zwitterion enhanced performance in palladium-phosphine catalyzed ethylene methoxycarbonylation

Zwitterions were used for the first time as promoters in ethylene methoxycarbonylation for the production of methyl propionate. They were found to improve the catalytic performance of the Pd–phosphine system. The presence of zwitterions could contribute to stabilize transition states and active catalytic Pd intermediates. The beneficial effect of the zwitterions was found to be most pronounced, when low amount of a strong acid (MeSO3H) was used with respect to palladium (below 2 equiv.). Under these conditions, phoshpine ligand alkylation and reaction vessel corrosion are also anticipated to be less severe.

General information
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Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Authors: Khokarale, S. G. (Intern), Garcia-Suarez, E. J. (Intern), Xiong, J. (Intern), Mentzel, U. V. (Intern), Fehrmann, R. (Intern), Riisager, A. (Intern)
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Scopus rating (2015): SJR 0.998 SNIP 1.129 CiteScore 3.55
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.162 SNIP 1.321 CiteScore 3.81
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.206 SNIP 1.283 CiteScore 3.6
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BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.165 SNIP 1.438 CiteScore 3.2
Absorption and oxidation of NO in ionic liquids

The present invention concerns the absorption and in situ oxidation of nitric oxide (NO) in the presence of water and oxygen in ionic liquid compositions at ambient temperature.

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Authors: Riisager, A. (Intern), Kunov-Kruse, A. J. (Intern), Mossin, S. (Intern), Fehrmann, R. (Intern)
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Accurate prediction of secondary metabolite gene clusters in filamentous fungi.

Biosynthetic pathways of secondary metabolites from fungi are currently subject to an intense effort to elucidate the genetic basis for these compounds due to their large potential within pharmaceutics and synthetic biochemistry. The preferred method is methodical gene deletions to identify supporting enzymes for key synthases one cluster at a time. In this study, we design and apply a DNA expression array for Aspergillus nidulans in combination with legacy data to form a
comprehensive gene expression compendium. We apply a guilt-by-association-based analysis to predict the extent of the biosynthetic clusters for the 58 synthases active in our set of experimental conditions. A comparison with legacy data shows the method to be accurate in 13 of 16 known clusters and nearly accurate for the remaining 3 clusters. Furthermore, we apply a data clustering approach, which identifies cross-chemistry between physically separate gene clusters (superclusters), and validate this both with legacy data and experimentally by prediction and verification of a supercluster consisting of the synthase AN1242 and the prenyltransferase AN11080, as well as identification of the product compound nidulanin A. We have used A. nidulans for our method development and validation due to the wealth of available biochemical data, but the method can be applied to any fungus with a sequenced and assembled genome, thus supporting further secondary metabolite pathway elucidation in the fungal kingdom.

**General information**

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Organisations: Department of Systems Biology, Center for Microbial Biotechnology, Center for Biological Sequence Analysis, Department of Chemistry, Organic Chemistry, Technical University of Denmark  
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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 (2016): CiteScore 8.56 SJR 6.321 SNIP 2.629  
Web of Science (2016): Indexed yes  
BFI (2015): BFI-level 2  
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Web of Science (2015): Indexed yes  
BFI (2014): BFI-level 2  
Scopus rating (2014): SJR 6.853 SNIP 2.725 CiteScore 8.86  
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Scopus rating (2013): SJR 6.989 SNIP 2.73 CiteScore 9.5  
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ISI indexed (2012): ISI indexed yes  
Web of Science (2012): Indexed yes  
BFI (2011): BFI-level 2  
Scopus rating (2011): SJR 6.771 SNIP 2.636 CiteScore 9.31  
ISI indexed (2011): ISI indexed yes  
Web of Science (2011): Indexed yes  
BFI (2010): BFI-level 2  
Scopus rating (2010): SJR 6.769 SNIP 2.529  
Web of Science (2010): Indexed yes  
BFI (2009): BFI-level 2  
Scopus rating (2009): SJR 6.913 SNIP 2.544  
Web of Science (2009): Indexed yes
Acid Gas Removal from Natural Gas with Alkanolamines: A Modeling and Experimental Study

Some 40% of the world’s remaining gas reserves are sour or acid, containing large quantities of CO₂ and H₂S and other sulfur compounds. Many large oil and gas fields have more than 10 mole % CO₂ and H₂S content. In the gas processing industry absorption with chemical solvents has been used commercially for the removal of acid gas impurities from natural gas. Alkanolamines, simple combinations of alcohols and ammonia, are the most commonly used category of chemical solvents for acid gas capture. This Ph.D. project is about thermodynamics of natural gas cleaning process with alkanolamines as solvent, modeling and experimental study. The project is collaboration between DTU and Statoil. Thermodynamic modeling is being done at DTU and experiments were performed at Statoil laboratories. In modeling part of the project, thermodynamic models were developed for CO₂-MDEA-H₂O, CO₂-MEA-H₂O, CO₂-MDEA-MEA-H₂O, H₂S-MDEA-H₂O, H₂SCH₄-MDEA-H₂O systems and the constituent binary subsystems of the mentioned mixtures. The experimental part of the project includes vapor-liquid equilibrium measurements for CO₂-MDEAH₂O and CO₂-MDEA-PZ-H₂O at atmospheric pressure, high pressure vapor-liquid equilibrium experiments for H₂S-CH₄-MDEA-H₂O, density measurements for aqueous MDEA and aqueous activated MDEA and piperazine solubility measurements in aqueous MDEA. Different commercial simulators together with the developed Extended UNIQUAC model were used to simulate the experimental data points. The effect of total pressure on acid gas solubility was also quantitatively investigated through both experimental and modeling approaches.

General Information
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Organisations: Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, Center for Energy Resources Engineering, Department of Chemistry
Authors: Sadegh, N. (Intern), Stenby, E. H. (Intern), Thomsen, K. (Intern)
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Main Research Area: Technical/natural sciences
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A Comparative Study of Reduced-Variables-Based Flash and Conventional Flash

For compositional transient simulations including compositional reservoir simulations, phase-equilibrium calculation, often formulated as a flash problem, can be time consuming. It is therefore important to speed up the calculation of phase equilibrium to improve the efficiency of the simulator. The reduced-variables methods, or the reduction methods, reformulate the original phase equilibrium problem with a smaller set of independent variables. Various versions of the reduced-variables methods have been proposed since the mid-1980s. The methods were first proposed for cubic equations of state (EOSs) with zero binary-interaction parameters (BIPs) and later generalized to situations with nonzero-BIP matrices. Most of the studies in the last decade suggest that the reduced-variables methods are much more efficient than the conventional flash method. However, Haugen and Beckner (2011) questioned the advantages of the reduced-variables methods in their recent paper. A fair comparison between the reduced-variables-based flash and the conventional flash is not straightforward because it is difficult to formulate the former as unconstrained minimization problems, and the flash calculation time is also related to the implementation quality. With the recent formulations by Nichita and Graciana (2011), it is possible to code the reduced-variables methods without extensive modifications of Michelsen’s conventional flash algorithm. A minimization-based reduced-variables algorithm was coded and compared with the conventional minimization-based flash. A test with the use of the SPE 3 example (Kenyon and Behie 1987) showed that the best reduction in time was less than 20% for the extreme situation of 25 components and just one row/column with nonzero BIPs. A better performance can be achieved by a simpler implementation directly using the sparsity of the BIP matrix.

General Information
State: Published
Organisations: Department of Chemistry, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, Center for Energy Resources Engineering, Technical University of Denmark
Authors: Yan, W. (Intern), Stenby, E. H. (Intern), Michelsen, M. L. (Intern)
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Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.01 SJR 0.95 SNIP 2.003
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.976 SNIP 1.838 CiteScore 2.37
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.185 SNIP 2.152 CiteScore 2.43
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.993 SNIP 1.773 CiteScore 2.25
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.047 SNIP 1.757 CiteScore 2.13
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.139 SNIP 1.757 CiteScore 2.3
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Aerobic dive limits of seals with mutant myoglobin using combined thermochemical and physiological data

This paper presents an integrated model of convective O$_2$-transport, aerobic dive limits (ADL), and thermochemical data for oxygen binding to mutant myoglobin (Mb), used to quantify the impact of mutations in Mb on the dive limits of Weddell seals (Leptonychotes weddellii). We find that wild-type Mb traits are only superior under specific behavioral and physiological conditions that critically prolong the ADL, action radius, and fitness of the seals. As an extreme example, the mutations in the conserved His-64 reduce ADL up to 14±2 min for routine aerobic dives, whereas many other mutations are nearly neutral in terms of ADL and the inferred fitness. We also find that the cardiac system, the muscle O$_2$-store, animal behavior (i.e. pre-dive ventilation), and the oxygen binding affinity of Mb, $K_{O_2}$, have co-evolved to optimize dive duration at routine aerobic diving conditions, suggesting that such conditions are mostly selected upon in seals. The model is capable of roughly quantifying the physiological impact of single-protein mutations and thus bridges an important gap between animal physiology and molecular (protein) evolution.

General information
State: Published
Organisations: Department of Chemistry, Physical and Biophysical Chemistry, Texas A&M University
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Scopus rating (2016): CiteScore 2.16 SJR 0.794 SNIP 0.879
A Mild Method for Regioselective Labeling of Aromatics with Radioactive Iodine

A novel technique to label ortho-, meta-, and para-trimethylsilyl-substituted aryl substituents with radioactive iodide is described. The method takes advantage of the ipso-directing and activating properties of trimethylsilyl substituents on the arenes. The method was demonstrated on a griseofulvin analogue with promising anticancer properties and on lidocaine, a widely used local anesthetic drug. Treatment of a trimethylsilyl precursor with Tl(OOCOCF3)3 followed by Na125I consistently afforded radioactive purities over 95 % in all cases.

General information

State: Published
Organisations: Department of Systems Biology, Department of Chemistry, Organic Chemistry, Center for Nanomedicine and Theranostics, Center for Microbial Biotechnology, University Hospital Heidelberg
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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Main Research Area: Technical/natural sciences

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Scopus rating (2016): CiteScore 8.86 SJR 2.564 SNIP 2.019
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Scopus rating (2014): SJR 2.398 SNIP 2.007 CiteScore 8.05
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Scopus rating (2013): SJR 2.266 SNIP 1.815 CiteScore 7.44
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Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 2.439 SNIP 1.709 CiteScore 6.64
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Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Antimony doped tin oxide modified carbon nanotubes as catalyst supports for methanol oxidation and oxygen reduction reactions

General information
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BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 8.46 SJR 3.037 SNIP 1.468
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
An Update on Lysine Deacylases Targeting the Expanding "Acylome"

Lysine e-amino acetylation has long been recognized as an epigenetically relevant post-translational modification of multiple residues in histone proteins. However, it has become clear that lysine acetylation is not restricted to histones, and therefore, it may be involved in the regulation of a wide variety of proteins, some of which have been identified and studied in detail. More recently, post-translational modifications of lysine side chains by additional acyl groups have also been identified, and some of these appear to be regulated by histone deacetylases (HDACs) and/or sirtuins. In this Concept, new Developments are discussed with emphasis on the enzymes that have been shown to catalyze the cleavage of these novel marks, including new assays and inhibitors. Ultimately, a deeper understand of these mechanisms should facilitate the development of ligands with therapeutic potential.
Aquatic toxicity testing of silver nanoparticles – a matter of timing

In recent years, the ecotoxicity of silver nanoparticles (AgNPs) has been studied intensively due to their high toxicity and extensive use in consumer products. However, the field of aquatic nanotoxicology is generally challenged by poor reproducibility, lack of dose-response relationships, and difficulties in controlling and/or describing the characteristics of the tested NPs. These issues may be related to the widespread approach of using freshly prepared stock solutions for ecotoxicity testing, as the introduction of NPs into aqueous media initiates time-dependent processes that possibly interfere with the toxicity testing, e.g. dissolution, speciation, aggregation, sedimentation and interactions with media components. The aim of this study was to investigate whether suspension of AgNPs in test media 24h prior to algal toxicity testing (a pre-suspension step) affects the toxicity and the reproducibility of the test. Ultimately, the aim is better control of the AgNPs in the algal test system and improved prerequisites for describing their toxicity to algae. The underlying hypothesis is that a large part in the variability of AgNPs toxicity to algae can be explained by the kinetics of dissolution and speciation of Ag ions in the test media. To reduce the amount of time in which changes to NPs may occur during testing, the exposure period was minimized. A recently proposed short-term (2h) algal test was applied, using 14C incorporation during photosynthesis as toxic endpoint [1]. For citrate coated spherical AgNPs with a nominal size of 30 nm, the resulting dose-response relationships from tests without (A) and with (B) the pre-suspension step are illustrated in figure 1. Without the pre-suspension step, poorly reproducible results were obtained and it was not possible to produce comparable EC50 values from the three test runs. Introduction of the presuspension step resulted in a higher degree of reproducibility and more comparable EC50 values, indicating better control of the processes affecting AgNPs during the 2h testing. Moreover, the algal toxicity of AgNPs increased when extending the pre-suspension step period from 24 to 48h, suggesting that ionic dissolution of AgNPs into the media takes part in AgNP toxicity. Our results stress the importance of dealing with the time-dependent processes that NPs undergo in aquatic media when investigating their toxicity.

General information
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Organisations: Department of Environmental Engineering, Department of Management Engineering, Department of Chemistry
Authors: Sørensen, S. N. (Intern), Owsianiak, M. (Intern), Engelbrekt, C. (Intern), Baun, A. (Intern)
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Main Research Area: Technical/natural sciences
Electronic versions: ICEENN_Abstract_Sara_Soerensen
Atomic scattering from an adsorbed monolayer solid with a helium beam that penetrates to the substrate

Diffraction and one-phonon inelastic scattering of a thermal energy helium atomic beam are evaluated in the situation that the target monolayer lattice is so dilated that the atomic beam penetrates to the interlayer region between the monolayer and the substrate. The scattering is simulated by propagating a wavepacket and including the effect of a feedback of the inelastic wave onto the diffracted wave, which represents a coherent re-absorption of the created phonons. Parameters are chosen to be representative of an observed p(1 × 1) commensurate monolayer solid of H2/NaCl(001) and a conjectured p(1 × 1) commensurate monolayer solid of H2/KCl(001). For the latter, there are cases where part of the incident beam is trapped in the interlayer region for times exceeding 50 ps, depending on the spacing between the monolayer and the substrate and on the angle of incidence. The feedback effect is large for cases of strong transient trapping. © 2013 American Institute of Physics.
Serotonin (5-hydroxytryptamine, 5-HT) is a prevalent neurotransmitter throughout the animal kingdom. It exerts its effect through the specific binding to the serotonin receptor, but recent research has suggested that neural transmission may
also be affected by its nonspecific interactions with the lipid matrix of the synaptic membrane. However, membrane–5-HT interactions remain controversial and superficially investigated. Fundamental knowledge of this interaction appears vital in discussions of putative roles of 5-HT, and we have addressed this by thermodynamic measurements and molecular dynamics (MD) simulations. 5-HT was found to interact strongly with lipid bilayers (partitioning coefficient ~1200 in mole fraction units), and this is highly unusual for a hydrophilic solute like 5-HT which has a bulk, oil–water partitioning coefficient well below unity. It follows that membrane affinity must rely on specific interactions, and the MD simulations identified the salt-bridge between the primary amine of 5-HT and the lipid phosphate group as the most important interaction. This interaction anchored cationic 5-HT in the membrane interface with the aromatic ring system pointing inward and a prevailing residence between the phosphate and the carbonyl groups of the lipid. The unprotonated form of 5-HT shows the opposite orientation, with the primary amine pointing toward the membrane core. Partitioning of 5-HT was found to decrease lipid chain order. These distinctive interactions of 5-HT and model membranes could be related to nonspecific effects of this neurotransmitter.
The purpose of this study was to identify and characterize fungal natural products (NPs) with in vitro bioactivity towards leukemia cells. We based our screening on a combined analytical and bio-guided approach of LC-DAD-HRMS dereplication, explorative solid-phase extraction (E-SPE), and a co-culture platform of CLL and stromal cells. A total of 289 fungal extracts were screened and we tracked the activity to single compounds in seven of the most active extracts. The novel ophiobolin U was isolated together with the known ophiobolins C, H, K as well as 6-epiophiobolins G, K and N from three fungal strains in the Aspergillus section Usti. Ophiobolins A, B, C and K displayed bioactivity towards leukemia cells with induction of apoptosis at nanomolar concentrations. The remaining ophiobolins were mainly inactive or only slightly active at micromolar concentrations. Dereplication of those ophiobolin derivatives possessing different activity in combination with structural analysis allowed a correlation of the chemical structure and conformation with the extent of bioactivity, identifying the hydroxy group at C3 and an aldehyde at C21, as well as the A/B-cis ring structure, as indispensable for the strong activity of the ophiobolins. The known compounds penicillic acid, viridicatumtoxin, calbistrin A, brefeldin A, emestrin A, and neosolaniol monoacetate were identified from the extracts and also found generally cytotoxic.
Biobrændsel - et varmt alternativ

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Authors: Frey, A. M. (Intern), Klerke, A. (Intern), Due-Hansen, J. (Intern), Christensen, C. H. (Intern)
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Biomass Conversion in Ionic Liquids - In-situ Investigations
Due to rising oil prices and global warming caused by CO2 emissions, there is an increased demand for new types of fuels and chemicals derived from biomass. This thesis investigates catalytic conversion of cellulose into sugars in ionic liquids and the important platform chemical 5-hydroxymethylfurfural (HMF). The thesis focuses on kinetic and mechanistic investigations using new in-situ FTIR spectroscopic methods based on the ATR-principle. At first the kinetics of cellulose hydrolysis and the simultaneously HMF formation was investigated in the ionic liquid 1-butyl-2,3-dimethylimidazolium chloride using sulfuric acid, solid acids and Lewis acidic chromium(III)chloride as catalysts. Initially the important glycosidic group vibration was located at 1155 cm\(^{-1}\). The new in-situ spectroscopic method successfully determined activation energies for hydrolysis to be 92-96 kJ/mol regardless of the catalyst used. The often used cellulose model cellobiose was found to hydrolyze substantially easier with an activation energy of only 69 kJ/mol. The activation energies of HMF formation could simultaneously be determined to be 84 and 102 kJ/mol for Brønsted and Lewis acid catalysis respectively. The low activation energies suggest that the ionic liquid acts co-catalytic by stabilizing the oxocarbenium transition state. The chromium catalyzed conversion of glucose to HMF in ionic liquid 1-butyl-3-methylimidazolium chloride with CrCl\(_3\)·6H\(_2\)O and CrCl\(_2\) as catalysts was investigated. The CrCl\(_3\)·6H\(_2\)O catalyst exhibited high initial conversion rates but suffered from pronounced product inhibition. The rates were 2-3 higher if water was removed simultaneously during reaction. Independent of whether water was present or not activation energies energies were found to be 100-102 kJ/mol. For CrCl\(_2\) the initial rates were around 8 times lower but the activation energy was identical the the ones found for CrCl\(_3\)·6H\(_2\)O. Thus the activity was attributed to around 12 % of chromium(III) that was found to present in the sample. The CrCl\(_3\) showed no sign of product inhibition and followed first order kinetics, which resulted in high conversion at longer reaction times compared to CrCl\(_3\)·6H\(_2\)O. In a proposed mechanism this was suggested to be due to a Cr\(^{II}/\)Cr\(^{III}\) synergy. A kinetic model based on active monomeric [CrCl\(_6\)]\(^{3-}\) species was proposed showing that the product inhibition resulted in second order like kinetic behavior. The fructose dehydration was investigated in both the presence and absence of CrCl\(_3\)·6H\(_2\)O. The partly dehydrated fructose intermediates were accumulated in the absence of chromium and water, leading to formation of humins. In the presence of CrCl\(_3\)·6H\(_2\)O the reaction was selective and the rates were 6-30 times higher with an activation energy of 74 kJ/mol. The thesis identifies the product inhibition as a major challenge for technical utilization of chromium catalysts in biomass conversion.

General information
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Organisations: Centre for Catalysis and Sustainable Chemistry, Department of Chemistry
Authors: Kunov-Kruse, A. J. (Intern), Fehrmann, R. (Intern), Riisager, A. (Intern)
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Main Research Area: Technical/natural sciences
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Brønsted acid ionic liquid catalyzed formation of pyruvaldehyde dimethylacetal from triose sugars
A series of sulfonic acid functionalized ionic liquids (SO\(_3\)H-ILs) have been synthesized, characterized and investigated as catalysts for the conversion of the triose sugars, 1,3-dihydroxyacetone (DHA) and glyceraldehyde (GLA), to pyruvaldehyde dimethylacetal (PADA) in methanol. Depending on the reaction conditions and the applied SO\(_3\)H-ILs a good yield of up to 52% of PADA was obtained. Under identical reaction conditions the derivative of PADA, 1,1,2,2-tetramethoxy propane (TMP), could be obtained in yields up to 49% using another SO\(_3\)H-IL.
Catalysis in Molten Ionic Media
This chapter deals with catalysis in molten salts and ionic liquids, which are introduced and reviewed briefly, while an in-depth review of the oxidation catalyst used for the manufacturing of sulfuric acid and cleaning of flue gas from electrical power plants is the main topic of the chapter. The historical development of the process during the last 100 years is described briefly; it is noteworthy that the liquid nature of the catalyst medium was not recognized before the early 1940s. The catalyst system appears quite complicated due to the complex nature of the melt components, which are not identified easily. It has been shown that the melt consists of vanadium oxosulfato complexes in the oxidation states III-V in an alkali pyrosulfate solvent. However, many basic data for alkali pyrosulfates and oxosulfato vanadates have turned out to be either nonexisting or unreliable. As a result, the fundamental research described in this chapter involves (i) the synthesis of compounds and pure chemicals; (ii) the determination of basic physical and chemical data as melting point, density, heat capacity, and so on; (iii) the construction of phase diagrams; (iv) the determination of the crystal structure of vanadium compounds, of which the majority are identified as catalyst deactivation products; and (v) studies of molecular structure and catalytic activity. Finally, the reaction mechanism is highlighted, which represents the state of the art of that catalytic process by 2013. © 2013 Elsevier Inc. All rights reserved.

Catalyst for the carboxylation of carbonylated compounds in the gas phase
The invention relates to a catalyst for the carboxylation of carbonylated compounds in the gas phase. Said catalyst consists of a metal complex which is active when the carboxylation is under reaction conditions and an organic salt, which is solid under normal conditions and liquid under reaction conditions, on the porous inert support material.
Catalytic conversion of lignocellulosic biomass using copper doped porous metal oxides

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Yale University
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Web of Science (2014): Indexed yes
Scopus rating (2013): SJR 0.101 SNIP 0.003
Web of Science (2013): Indexed yes
Scopus rating (2012): SJR 0.1 SNIP 0
Scopus rating (2011): SJR 0.101 SNIP 0
Web of Science (2011): Indexed yes
Scopus rating (2010): SJR 0.101 SNIP 0
Scopus rating (2009): SJR 0.101 SNIP 0
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.101 SNIP 0
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.101 SNIP 0
Scopus rating (2006): SJR 0.101
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.101
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.104 SNIP 0.028
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 0.111 SNIP 0.008
Scopus rating (2002): SJR 0.115 SNIP 0.046
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.111 SNIP 0.038
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 0.111
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Publication: Research - peer-review › Conference abstract in journal – Annual report year: 2013

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**

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- 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
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- 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
- Web of Science (2010): Indexed yes
Original language: English
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Source: dtu
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Publication: Research - peer-review › Journal article – Annual report year: 2012

**Cationic liposomal drug delivery system for specific targeting of human cd14+ monocytes in whole blood**

This invention concerns a liposome comprising lipids and at least one active ingredient, wherein at least one of the lipids is a cationic lipid; said liposome exhibiting a net positive charge at physiological conditions at which said liposome preferentially adheres to monocytes in freshly drawn blood when compared to adherence to granulocytes, T-lymphocytes, B-lymphocytes and/or NK cells in freshly drawn blood, to a lipid-based pharmaceutical composition comprising said liposomes and their use in monocytic associated prophylaxis, treatment or amelioration of a condition such as cancer, an
infectious disease, an inflammatory disease, an autoimmune disease or allergy.

**General information**

**State:** Published

**Organisations:** Department of Micro- and Nanotechnology, Colloids and Biological Interfaces, Department of Chemistry, Physical and Biophysical Chemistry

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**Publication date:** 2013

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Main Research Area: Technical/natural sciences

**Characterization of Cu-exchanged SSZ-13: a comparative FTIR, UV-Vis, and EPR study with Cu-ZSM-5 and Cu-β with similar Si/Al and Cu/Al ratios**

Cu-SSZ-13 has been characterized by different spectroscopic techniques and compared with Cu-ZSM-5 and Cu-β with similar Si/Al and Cu/Al ratios and prepared by the same ion exchange procedure. On vacuum activated samples, low temperature FTIR spectroscopy allowed us to appreciate a high concentration of reduced copper centres, i.e. isolated Cu+ ions located in different environments, able to form Cu+(N2), Cu+(CO)n (n = 1, 2, 3), and Cu+(NO)n (n = 1, 2) upon interaction with N2, CO and NO probe molecules, respectively. Low temperature FTIR, DRUV-Vis and EPR analysis on O2 activated samples revealed the presence of different Cu2+ species. New data and discussion are devoted to (i) [Cu–OH]+ species likely balanced by one framework Al atom; (ii) mono(μ-oxo)dicopper [Cu2(μ-O)]2+ dimers observed in Cu-ZSM-5 and Cu-β, but not in Cu-SSZ-13. UV-Vis-NIR spectra of O2 activated samples reveal an intense and finely structured d–d quadruplet, unique to Cu-SSZ-13, which is persistent under SCR conditions. This differs from the 22 700 cm⁻¹ band of the mono(μ-oxo)dicopper species of the O2 activated Cu-ZSM-5, which disappears under SCR conditions. The EPR signal intensity sets Cu-β apart from the others.

**General information**

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Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, University of Turin, Haldor Topsoe AS, Technical University of Denmark

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Filamentous fungi and other microorganisms have amazing abilities to synthesize structural complex, diverse and unique small organic molecules. Many are bioactive and numerous compounds such as mycotoxins, antifungal, and anticancer agents have been reported in the literature within the last more than 100 years. New natural products (NPs) are continually discovered and with the increase in selective biological assays, previously described compounds often also display novel bioactivities, justifying their presence in novel screening efforts. Screening and discovery of compounds with activity towards chronic lymphocytic leukemia (CLL) cells is crucial since CLL is considered as an incurable disease. To discover novel agents that targets CLL cells is complicated. CLL cells rapidly undergo apoptosis in vitro when they are removed from their natural microenvironment, even though they are long-living cells in vivo. Fortunately viability of CLL
cells can be maintained in vitro by co-cultivation with stromal cells mimicking in vivo conditions. This has led to the development of a co-culture assay that is ideally suited for screening of NPs. The main goal of this study has been to discover fungal NPs with activity towards CLL cells in vitro. We based our screening on a combined analytical and bio-guided approach of LC-DADHRMS based dereplication, explorative solid-phase-extraction (E-SPE), and a co-culture platform of CLL and stromal cells. The activity was tracked to single compounds in seven of the most active extracts in a screening setup including 289 fungal extracts. The novel ophiobolin U was isolated together with the known ophiobolin C, H, K as well as 6-epiophiobolin G, K and N from three fungal strains in the Aspergillus section Usti, and further ophiobolins were bought from commercial sources. Ophiobolin A, B, C and K induced apoptosis in CLL cells with LC50 values of values of 1, 2, 8, and 4 nM, respectively, with a possible narrow therapeutic window. The remaining ophiobolins were inactive. Eight other bioactive extracts were addressed and the compounds responsible for the activity towards CLL cells were identified from six of the extracts. The known compounds: penicillic acid, viridicatumtoxin, calbistrin A, brefeldin A, emestrin A, and neosolaniol monoaacetate all displayed activity towards CLL cells though they all showed general cytotoxic in the assay. In the remaining two extracts the bioactive compounds were tentatively identified as cyclostrepentine E and a compound belonging to the statin family of compounds though these results are inconclusive.

A second aim of this PhD project has been to discover novel bioactive NPs using a target-guided approach based on MS and NMR. In one project a target-guided approach based on MS lead to isolation of two new cytochalasins, sclerotionigrin A and B and the known proxiphostin from the fungal species Aspergillus sclerotieoniger. The compounds are moderately cytotoxic towards CLL. In a second approach three novel bioactive micropeptins produced by cyanobacteria were discovered through target-guided isolation based on NMR. The micropeptins displayed inhibitory activity towards serine proteases: chymotrypsin and elastase with IC50 values between 5.9 and 28.0 μM.

In conclusion, this PhD study adds to the knowledge of bioactive NPs produced by filamentous fungi, and in particular activity towards CLL cells. The results obtained here have been based on the use of a combined bio-guided and analytical dereplication approach. This PhD study also includes a review of 50 compounds or compound families with anticancer activity primarily produced by Aspergillus, Penicillium and Talaromyces.

General information
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Organisations: Department of Systems Biology, Natural Product Chemistry, Department of Chemistry, Organic Chemistry
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Clearance of Pseudomonas aeruginosa Foreign-Body Biofilm Infections through Reduction of the Cyclic Di-GMP Level in the Bacteria
Opportunistic pathogenic bacteria can engage in biofilm-based infections that evade immune responses and develop into chronic conditions. Because conventional antimicrobials cannot efficiently eradicate biofilms, there is an urgent need to develop alternative measures to combat biofilm infections. It has recently been established that the secondary messenger cyclic diguanosine monophosphate (c-di-GMP) functions as a positive regulator of biofilm formation in several different bacteria. In the present study we investigated whether manipulation of the c-di-GMP level in bacteria potentially can be used for biofilm control in vivo. We constructed a Pseudomonas aeruginosa strain in which a reduction in the c-di-GMP level can be achieved via induction of the Escherichia coli YhjH c-di-GMP phosphodiesterase. Initial experiments showed that induction of yhjH expression led to dispersal of the majority of the bacteria in in vitro-grown P. aeruginosa biofilms. Subsequently, we demonstrated that P. aeruginosa biofilms growing on silicone implants, located in the peritoneal cavity of mice, dispersed after induction of the YhjH protein. Bacteria accumulated temporarily in the spleen after induction of biofilm dispersal, but the mice tolerated the dispersed bacteria well. The present work provides proof of the concept that modulation of the c-di-GMP level in bacteria is a viable strategy for biofilm control.

General information
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Organisations: Department of Chemistry, Organic Chemistry, University of Copenhagen
Complexity of gold nanoparticle formation disclosed by dynamics study

Although chemically synthesized gold nanoparticles (AuNPs) from gold salt (HAuCl₄) are among the most studied nanomaterials, understanding the formation mechanisms is a challenge mainly due to limited dynamics information. A range of in situ methods with down to millisecond (ms) time resolution have been employed in the present report to monitor time-dependent physical and chemical properties in aqueous solution during the chemical synthesis. Chemical synthesis of AuNPs is a reduction process accompanied by release of ions and protons, and formation of solid particles. Dynamic information from redox potential, pH, conductivity, and turbidity of the solution enables distinct observation of reduction and nucleation/growth of AuNPs phases. The dynamics of the electrochemical potential shows that reduction of gold salt (HAuCl₄ and its hydrolyzed forms) occurs via intermediate [AuCl₂]⁻ to form Au atoms during the early stage of the synthesis process. pH- and conductivity-dynamics point further clearly to formation of coating layers on AuNPs and adsorbate exchange between MES and starch. © 2013 American Chemical Society.
Computational Approach to Electron Charge Transfer Reactions

The step from ab initio atomic and molecular properties to thermodynamic - or macroscopic - properties requires the combination of several theoretical tools. This dissertation presents constant temperature molecular dynamics with bond length constraints, a hybrid quantum mechanics-molecular mechanics scheme, and tools to analyse statistical data and generate relative free energies and free energy surfaces. The methodology is applied to several charge transfer species and reactions in chemical environments - chemical in the sense that solvent, counter ions and substrate surfaces are taken in to account - which directly influence the reactants and resulting reaction through both physical and chemical interactions. All methods are though general and can be applied to different types of chemistry. First, the basis of the various theoretical tools is presented and applied to several test systems to show general (or expected) properties. Properties such as in the physical and (semi-)chemical interface between classical and quantum systems and the effects of molecular bond length constraints on the temperature during simulations. As a second step the methodology is applied to the symmetric and asymmetric charge transfer reactions between several first-row transition metals in water. The results are compared to experiments and rationalised with classical analytic expressions. Shortcomings of the methods are accounted for with clear steps towards improved accuracy. Later the analysis is extended to more complex systems composed of a larger osmium complex in solution and at the solute-substrate interfaces, where in particular the redox state of the complex is controlled through chemical means. The efficiency of the hybrid-classical and quantum mechanics method is used to generate adequate statistics and a simple post-sampling scheme used to generate free energy surfaces - which compare to full ab initio calculations. In the last part both the molecular dynamics and hybrid classical and quantum mechanics method are used to generate a vast data set for the accurate analysis of dynamical structure modes. This is for a large iridium-iridium dimer complex which shows a dramatic structural (and vibrational) change upon electronic excitation.

General information
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Organisations: Center for Atomic-scale Materials Design, Department of Physics, Department of Chemistry, NanoChemistry
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Original language: English
Main Research Area: Technical/natural sciences
Computational Enzymology, a ReaxFF approach
This PhD project essay is about the development of a new method to improve our understanding of enzyme catalysis with atomistic details. Currently the theory able to describe chemical systems and their reactivity is quantum mechanics (QM): electronic structure methods that use approximations of QM theory to describe molecular structure. Modeling enzyme reactions is anyway still inaccessibile to these methods because the size of the problem would result in many-particle equations too complicated to be solved even with rather crude approximations such as Hartree-Fock (HF). At the same time there are ordinary classical models - the molecular mechanics (MM) force-fields - that use newtonian mechanics to describe molecular systems. At this level it is possible to include the entire enzyme system still having light equations but renouncing to an easy modeling of chemical transformation during the simulation time. In short: on one hand we have accurate QM methods able to describe reactivity but limited in the size of the system to describe, while on the other hand we have molecular mechanics and ordinary force-fields that are virtually unlimited in size but unable to straightforwardly describe chemical reactivity. A reactive force-field (ReaxFF) is a simplified model that aims to bridge the gap between quantum chemistry methods to the ordinary force-fields of the classical molecular mechanics methods, enabling MM to model chemical reactions as a QM method with bond forming and breaking events during the simulation time. This has been accomplished by simply introducing anharmonicities in the potential energy terms of the force-field. Starting from a published ReaxFF force-field developed for modeling glycine aminoacid a novel ReaxFF force-field, ProtReaxFF, has been developed, optimized and applied to enzyme catalysis reactions.

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Organisations: Department of Chemistry, Organic Chemistry
Authors: Corozzi, A. (Intern), Fristrup, P. (Intern)
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Publication date: 2013

Conformational analysis of Gly-Ala-NHMe in D$_2$O and DMSO solutions: A two-dimensional infrared spectroscopy study
A relevant number of experiments on short peptides has been performed in recent years. One of the major problems rises from the simultaneous presence of slightly different conformers at equilibrium in solution. In the present paper, the conformational characteristics of the Gly-l-Ala-Methyl amide dipeptide in D2O and DMSO solutions are investigated by nonlinear IR spectroscopy. The pump-probe scheme with ultrashort mid-infrared pulses, in the Amide I region, is used to determine the mutual orientation of the two C=O bonds and the dynamics due to solute-solvent interactions. The coupling between Amide I modes is evaluated from both linear and 2D spectra. The interconversion between the different conformations occurs on time scales longer than the vibrational lifetime, and the spectral diffusion observed in 2D spectra is attributed to the solvent dynamics. Quantum mechanical calculations and molecular dynamics simulations are performed to identify the most stable geometries. By comparing the experimental and the theoretical data, we establish the prevalence of β-like polar conformers in both water and DMSO solvents. © 2013 American Chemical Society.

General information
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Organisations: Department of Chemistry, Organic Chemistry, Heriot-Watt University, Scuola Normale Superiore di Pisa, National Research Council of Italy, Università di Pisa, Università degli Studi di Firenze, University of Perugia
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Consistent descriptions of metal–ligand bonds and spin-crossover in inorganic chemistry

Density functional theory (DFT) is today the unchallenged tool for routinely obtaining molecular information on chemical stability, reactivity, and electronic structure across the Periodic Table. The chemical bond is the fundamental unit of molecular structure and reactivity, and thus, large-scale DFT studies of inorganic systems in catalysis and bioinorganic chemistry rely directly on the ability to balance correlation effects in the involved bonds across the s-, p-, and d-blocks. This review concerns recent efforts to describe such bonds accurately and consistently across the s-, p-, and d-blocks. Physical effects and ingredients in functionals, their systematic errors, and approaches to deal with them are discussed, in order to identify broadly applicable methods for inorganic chemistry.
Copper(II)–imida‐salen Complexes Encapsulated into NaY Zeolite for Oxidations Reactions

The oxidation of phenol, cyclohexanol and hydroquinone has been screened in the presence of copper(II) complexes with the Schiff‐base salen ligand, 1,5-bis[(E)-5-chloro-2-hydroxybenzylimidemeneamino]-1H-imidazole-4-carbonitrile, and encapsulated into NaY zeolite by using two different methods. The new heterogeneous catalysts were characterized by SEM, XRD, FTIR, EPR and Raman spectroscopy as well as by chemical analysis. The structures of the copper(II) complexes were proposed on the basis of theoretical studies (DFT). The catalytic activities of the encapsulated copper(II) complexes in NaY were compared with their homogeneous counterparts. The results show higher or similar substrate conversion when compared with the free complex in all the reactions tested. After their use in catalytic reaction, these catalysts were found to be reusable without loss of activity.

General information
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Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, University of Minho, Catalytic Spectroscopy Laboratory, Universidade do Porto
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The metallonuclease colicin E7 is a member of the HNH family of endonucleases. It serves as a bacterial toxin in *Escherichia coli*, protecting the host cell from other related bacteria and bacteriophages by degradation of their chromosomal DNA under environmental stress. Its cell-killing activity is attributed to the nonspecific nuclease domain (NColE7), which possesses the catalytic ββα-type metal ion-binding HNH motif at its C-terminus. Mutations affecting the positively charged amino acids at the N-terminus of NColE7 (444-576) surprisingly showed no or significantly reduced endonuclease activity [Czene et al. (2013), J. Biol. Inorg. Chem. 18, 309-321]. The necessity of the N-terminal amino acids for the function of the C-terminal catalytic centre poses the possibility of allosteric activation within the enzyme. Precise knowledge of the intramolecular interactions of these residues that affect the catalytic activity could turn NColE7 into a novel platform for artificial nuclease design. In this study, the N-terminal deletion mutant ΔN4-NColE7-C* of the nuclease domain of colicin E7 selected by *E. coli* was overexpressed and crystallized at room temperature by the sitting-drop vapour-diffusion method. X-ray diffraction data were collected to 1.6 Å resolution and could be indexed and averaged in the trigonal space group *P*3121 or *P*3221, with unit-cell parameters *a* = *b* = 55.4, *c* = 73.1 Å. Structure determination by molecular replacement is in progress.

**Crystallization and preliminary crystallographic analysis of an *Escherichia coli*-selected mutant of the nuclease domain of the metallonuclease colicin E7**

**General information**

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**Organisations:** Department of Chemistry, Metalloprotein Chemistry and Engineering, University of Szeged, MTA-SZTE Bioinorganic Chemistry Research Group, University of Tsukuba, University of Copenhagen
Cu catalyzed oxidation of 5-hydroxymethylfurfural to 2,5-diformylfuran and 2,5-furandicarboxylic acid under benign reaction conditions

The renewable chemical building block 5-hydroxymethylfurfural (HMF) was oxidized to 2,5-diformylfuran by an oxidation system consisting of the radical 2,2,6,6-tetramethyl-piperidin-1-oxyl (TEMPO) and CuCl. The system was optimized by exploring several reaction conditions and by employing nitrogen containing promoters (NCPs) to obtain excellent yields. In acetonitrile a 95% DFF yield was obtained after 24h with ambient pressure of dioxygen at room temperature in the presence of different NCPs, which – to our knowledge – is the best result reported thus far for this reaction. The use of NCPs made it further possible to apply various traditional solvents, e.g. acetone, methanol and methyl isobutyl ketone for the reaction. The latter can be used as extraction solvent for HMF synthesis in aqueous media and thus integrate the two
processes. Additionally, HMF was oxidized to 2,5-furandicarboxylic acid by a modified oxidation protocol consisting of CuCl and t-BuOOH. In all the reactions, mild conditions, including room temperature were employed.
Deactivation in Continuous Deoxygenation of C18-Fatty Feedstock over Pd/Sibunit

Catalytic continuous deoxygenation of stearic acid, ethyl stearate and tristearin without any solvents was investigated using Pd/Sibunit as a catalyst in a trickle bed reactor at 300 °C. The main emphasis was to investigate the effect of gas atmosphere and catalyst deactivation. In addition to liquid-phase analysis made offline by GC, also online gas-phase analysis with IR were performed. The main liquid-phase product coming from all reactants was n-heptadecane. In addition to deoxygenation, which was observed for all substrates, also C18 and C16 alkanes were formed from tristearin. The relative ratios between stearic acid, ethyl stearate and tristearin conversions to alkanes after 3 days time-on-stream were 2.8/2.3/1.0, respectively using 5 % H2/Ar as a gas atmosphere, whereas rapid catalyst deactivation occurred with all substrates under H2-lacking atmosphere. The spent catalyst’s specific surface area profile along the downward reactor was maximum in the middle of the catalyst beds with the highest pore shrinking in the beginning and at the end of the reactor catalyst segments in the case of stearic acid and tristearin deoxygenation whereas that decreased consecutively as ethyl stearate passed through the reactor.

General information

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Scopus rating (2014): SJR 0.989 SNIP 0.862 CiteScore 2.29
The present thesis revolves around the challenges involved in removal of nitrogen oxides in biomass fired power plants. Nitrogen oxides are unwanted byproducts formed to some extent during almost any combustion. In coal fired plants these byproducts are removed by selective catalytic reduction, however the alkali in biomass complicate matters. Alkali in biomass severely deactivates the catalyst used for the selective catalytic reduction in matter of weeks, hence a more alkali resistant catalyst is needed. In the thesis a solution to the problem is presented, the nano particle deNOx catalyst. Through the thesis the one-pot sol-gel synthesis of this nano particle catalyst, have been optimised by evaluation of each synthesis step. Resulting in a highly active catalyst comprising amorphous vanadia on a high surface area crystalline anatase carrier. Due to the high surface area, loadings of 20 wt.% vanadia could be obtained without exceeding the V2O5 monolayer coverage. Explaining the very high activity corresponding to a factor of 2, compared to an industrial reference. Even at high vanadia loadings the catalyst did not show any sign of increased SO2 oxidation, compared with a low vanadia industrial reference catalyst. Furthermore long-term activity measurements at normal operating temperature
revealed that the catalyst did not display any sign of deactivation. The catalyst showed very high resistance towards potassium poisoning maintaining a 16 times higher activity than the equally poisoned industrial reference catalyst, after impregnation of 225 mole potassium/g of catalyst. A catalyst plate was synthesised using 20 wt.% sepiolite mixed with nano catalyst, supported by a SiO2-fibre mesh. Realistic potassium poisoning was performed on the catalyst plate, by exposure in a potassium aerosol for 632 hours at 350 C. Owing to physical blocking of potassium by sepiolite fibres the composite catalyst showed a further increase in potassium resistance compared with the unsupported catalyst. Finally a refined mechanism was proposed for the nano particle SCR catalyst explaining insitu FTIR observation done on the system. Most importantly it indicated that the V=O bond did not break during the SCR reaction, suggesting that another oxygen is responsible for the activity of the active vanadia site.
Detection of the quorum sensing signal molecule N-Dodecanoyl-DL-homoserine lactone below 1 nanomolar concentrations using surface enhanced Raman spectroscopy

To the best of our knowledge we here for the first time demonstrate surface enhanced Raman spectroscopy (SERS) to detect a quorum sensing (QS) signal molecule below 1 nM concentration in both ultrapure water and under physiological conditions. Based on our results, SERS shows promise as a highly suitable tool for in situ measurements of low Acyl-Homoserine Lactone (AHL) concentrations in biofilms containing QS bacteria. Signal molecules communicate information about their environment and coordinate certain physiological activities in QS systems that exist in many bacteria. SERS enables detection of different AHLs at low concentrations due to structural differences observed in the corresponding SERS spectra. Ag colloidal nanoparticles, produced by the hydroxylamine reducing method, were used for the SERS measurements. SERS spectra of C12-HSL suspended in ultrapure water and in supplemented minimal medium were collected for 5 concentrations ranging from 2 μM to 0.2 nM, and a comparison between the spectra from these two media is also presented. We have been able to detect biologically relevant concentrations of AHL molecules ranging from 1 nM to 1 μM using SERS.

Development of a cysteine-deprived and C-terminally truncated GLP-1 receptor

The glucagon-like peptide-1 receptor (GLP-1R) belongs to family B of the G-protein coupled receptors (GPCRs), and has become a promising target for the treatment of type 2 diabetes. Here we describe the development and characterization of a fully functional cysteine-deprived and C-terminally truncated GLP-1R. Single cysteines were initially substituted with alanine, and functionally redundant cysteines were subsequently changed simultaneously. Our results indicate that Cys174, Cys226, Cys296 and Cys403 are important for the GLP-1-mediated response, whereas Cys236, Cys329, Cys341, Cys347, Cys438, Cys458 and Cys462 are not. Extensive deletions were made in the C-terminal tail of GLP-1R in order to determine the limit for truncation. As for other family B GPCRs, we observed a direct correlation between the length of the C-terminal tail and specific binding of 125I-GLP-1, indicating that the membrane proximal part of the C-terminal is involved in receptor expression at the cell surface. The results show that seven cysteines and more than half of the C-terminal tail can be removed from GLP-1R without compromising GLP-1 binding or function.
The increasing concerns for using phthalates have led to the discovery of the safer alternative Grindsted® SOFT-N-SAFE (SNS) by Dansico A/S (now known as DuPont Nutrition Biosciences Aps). The main component of SNS is based on acetylated glycerol monostearate, originating from hydrogenated castor oil. SNS is a 1-1 replacement alternative to the phthalate di(2-ethylhexyl)phthalate (DEHP). This alternative is, however, too expensive to be an actual alternative to phthalates, because of the expensive starting material castor oil and the use of acetic anhydride as acetylation reagent.
Besides this, the starting material is not very accessible, meaning that even if the production price of SNS was comparable to the production price of phthalates, SNS could not be produced in large enough quantities to replace the use DEHP. An alternative to SNS, the SNS-analogue (SNS-A), was suggested from glycerol monooleate originating from sunflower oil. Sunflower oil is less expensive and more accessible compared to castor oil and the SNS-A has been tested to have the same plasticizing effect and non-toxic effects as SNS. However, a sustainable and cheap way of synthesizing SNS-A has not been developed. The aim of this project was to find an alternative, sustainable and cheap synthetic pathway for the SNS-A in collaboration with DuPont Nutrition Biosciences Aps, Danish National Food institute (DTU-Food), Department of Engineering at Aarhus University (AU) and other group members from the Centre for Catalysis and Sustainable Chemistry at Department of Chemistry at Department of Chemistry at Technical University of Denmark (DTU-Chemistry). A three step synthetic pathway consisting of epoxidation, hydrogenation and acetylation of glycerol monooleate was early in the project suggested as the best procedure, and the different parts were divided between the parties in the project. This PhD project had three parts. The first part was to find an ionic liquid (IL) which could separate out the product from the reaction mixture and that could function as reaction media for one or more steps in the process. The second step was developing an epoxidation procedure and the third part was developing a hydrogenation method. The idea with using an IL as a reaction media and for product separation was also to a keep any water from the glycerol backbone of the material to avoid hydrolysis. This could be done by choosing an IL non-miscible with water, like the ones having a bis(trifluoromethylsulfonyl)amide anion. From the ILs synthesized or purchased it was not possible to find an IL which could separate out SNS. Several of the tested ILs could, however, be used as separation media after epoxidation or hydrogenation. Only one IL was miscible with the starting material and the epoxide but not the product from the hydrogenation, and all ILs where separation was possible after epoxidation step was non-miscible with the starting material. It was therefore not possible, from the ILs described here, to have a homogeneous reaction media for epoxidation with separation possible after this step. The second part of this study, the work with developing an epoxidation procedure, can be divided into two parts. The first epoxidation method was catalytic epoxidation in ILs where product separation was possible using a heteropoly acid based catalyst and hydrogen peroxide as oxidant. The IL giving the best result was N-butyl-N-methyl imidazolium bis(trifluoromethyl-sulfonyl)amide (abbreviated [BMIm][Tf2N]) and the epoxidation reaction was further investigated and optimized using this IL. Applying different reaction conditions resulted twice in a good epoxidation results, with conversions of 67 % and 70 % respectively. This, however, was not a sufficiently good result for up scaling of the process and reproducibility proved difficult. Accordingly, this method was abandoned. The epoxidation procedure was also tested with peracetic acid with acetic acid as both solvent and by-product from the reaction. Both substrate and product are soluble in the reaction media, but as acetic acid was to be added for the final acetylation step, this did not require a solvent removal step. Already in the initial experiments this system performed very promising, and the reaction was optimized with respect to the temperature, addition time and rate of peracetic acid and substrate concentration i.e. amount of solvent. Furthermore, the effect of water concentration was also investigated. After optimization, the result was satisfying as no large excess of peracetic acid needed to be used. The conversion rate was high at low temperatures, giving a short reaction time, and the amount of by-product low. The reproducibility of this reaction was high and it was tested many times in up to 2 L scale with the same satisfying result. Two methods for hydrogenation of the epoxide to the mono-hydroxy compound examined, a catalytic transfer hydrogenation (CTH) using a hydrogen donor and the use of molecular hydrogen gas. CTH was conducted with selected substrates or with the epoxide of interest in this project. Several solvents, many of them ILs, were tested with three different hydrogen donors and three different catalysts, known to be efficient in CTH reactions. However, no satisfying results were obtained using CTH as a hydrogenation method. Using molecular hydrogen gas for hydrogenation also resulted in problems. The hydrogenation of the epoxide obtained from epoxidation with peracetic acid gave mainly the saturated monoglyceride instead of the mono-hydroxy compound as intended. Several heterogeneous metal catalysts and reaction conditions were tested, but it was not possible to find a suitable method for the hydrogenation. Overall, this PhD study has established a potentially industrially viable epoxidation protocol as part of a new reaction pathway for the synthesis of SNS-A.
Direct measurement and modulation of single-molecule coordinative bonding forces in a transition metal complex.
Coordination chemistry has been a consistently active branch of chemistry since Werner’s seminal theory of coordination compounds inaugurated in 1893, with the central focus on transition metal complexes. However, control and measurement of metal-ligand interactions at the single-molecule level remain a daunting challenge. Here we demonstrate an interdisciplinary and systematic approach that enables measurement and modulation of the coordinative bonding forces in a transition metal complex. Terpyridine is derived with a thiol linker, facilitating covalent attachment of this ligand on both gold substrate surfaces and gold-coated atomic force microscopy tips. The coordination and bond breaking between terpyridine and osmium are followed in situ by electrochemically controlled atomic force microscopy at the single-molecule level. The redox state of the central metal atom is found to have a significant impact on the metal-ligand interactions. The present approach represents a major advancement in unravelling the nature of metal-ligand interactions and could have broad implications in coordination chemistry.

General information
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Organisations: NanoChemistry, Department of Chemistry, Department of Physics, Theoretical Atomic-scale Physics, Chalmers University of Technology, Chinese Academy of Sciences
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Discovery and Perspectives of Zeolite Sn-Beta
**Discovery of a novel selective PPARγ ligand with partial agonist binding properties by integrated in silico / in vitro work flow**

Full agonists to the peroxisome proliferator-activated receptor (PPAR)γ, such as Rosiglitazone, have been associated with a series of undesired side effects, such as weight gain, fluid retention, cardiac hypertrophy, and hepatotoxicity. Nevertheless, PPARγ is involved in the expression of genes that control glucose and lipid metabolism and is an important target for drugs against type 2 diabetes, dyslipidemia, atherosclerosis, and cardiovascular disease. In an effort to identify novel PPARγ ligands with an improved pharmacological profile, emphasis has shifted to selective ligands with partial agonist binding properties. Toward this end we applied an integrated in silico/in vitro workflow, based on pharmacophore- and structure-based virtual screening of the ZINC library, coupled with competitive binding and transactivation assays, and adipocyte differentiation and gene expression studies. Hit compound 9 was identified as the most potent ligand (IC50 = 0.3 μM) and a relatively poor inducer of adipocyte differentiation. The binding mode of compound 9 was confirmed by molecular dynamics simulation, and the calculated free energy of binding was -8.4 kcal/mol. A novel functional group, the carbonitrile group, was identified to be a key substituent in the ligand-protein interactions. Further studies on the transcriptional regulation properties of compound 9 revealed a gene regulatory profile that was to a large extent unique, however functionally closer to that of a partial agonist. © 2013 American Chemical Society.
Distribution of MEG and methanol in well-defined hydrocarbon and water systems: Experimental measurement and modeling using the CPA EoS

Liquid-liquid equilibria data for two binary and two ternary systems are reported in the temperature range of 303.15-323.15 K at atmospheric pressure. The binary systems measured are n-nonane + MEG and ethylbenzene + MEG and the ternary systems are n-nonane + MEG + water and ethylbenzene + MEG + water. These data are satisfactorily correlated (binaries) and predicted (ternaries) using Cubic Plus Association (CPA) equation of state (EoS). CPA is also applied to binary LLE of aromatic hydrocarbon + water and VLE of methane + methanol. Finally the distribution of water and inhibitors (methanol and MEG) in various phases is modeled using CPA. The hydrocarbon phase consists of mixture-1 (methane, ethane, n-butane) or mixture-2 (methane, ethane, propane, n-butane, n-heptane, toluene and n-decane). CPA can satisfactorily predict the water content in the gas phase of the multicomponent systems containing mixture-1 over a range of temperatures and pressures. Similarly the methanol content in the gas phase of mixture-1 + water + methanol systems is predicted satisfactorily with accuracy within experimental uncertainty. For VLE of mixture-2 + water + mixture-2 + MEG + water and mixture-2 + methanol + water systems, the organic phase compositions are satisfactorily predicted whereas modeling results are relatively less satisfactory for the vapor phase compositions partially due to uncertainties in the experimental data. © 2012 Elsevier B.V.
Does Pelletizing Catalysts Influence the Efficiency Number of Activity Measurements? Spectrochemical Engineering Considerations for an Accurate Operando Study

Porosity is a factor affecting catalyst efficiency in pelleted form. This implies that care should be taken with uncritically relating activity measurements from transmission operando FTIR to final catalyst performance. If the pelletizing pressure is excessive, a destruction of the pore structure of, for example, support oxides might take place, which in turn affects the pore size distribution and the porosity of the catalyst, leading to the observation of lower activity values due to decreased catalyst efficiency. This phenomenon can also apply to conventional activity measurements, in the cases that pelletizing and recrushing of samples are performed to obtain adequate particle size fractions for the catalytic bed. A case study of an operando investigation of a V2O3-WO3/TiO2-sepiolite catalyst is used as an example, and simple calculations of the influence of catalyst activity and internal pore diffusion properties are considered in this paper for the evaluation of catalyst performance in, for example, operando reactors. Thus, it is demonstrated that with a pelletizing pressure of

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General information
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Effects of mannose, fructose, and fucose on the structure, stability, and hydration of lysozyme in aqueous solution
The bio-protective properties of monosaccharides, namely mannose, fructose and fucose, on the stability and dynamical properties of the NMR determined hen egg-white lysozyme structure have been investigated by means of molecular dynamics simulations at room temperature in aqueous solution and in 7 and 13 wt % concentrations of the three sugars. Results are discussed in the framework of the bio-protective phenomena. The three sugars show similar bio-protective behaviours at room temperature (300 K) in the concentration range studied as shown by the small RMSDs of the resulting MD structures from that of starting NMR structure. The effects of sugars on protein conformation are found to be relatively strong in that the conformation of lysozyme is stable after an initial 9 ns equilibration for fucose and mannose and 12 ns equilibration for fructose, respectively, at high concentrations. For mannose the final RMSD is significantly smaller than that of fucose and fructose at the higher concentration, while at the lower concentration the RMSD are essentially the same. The radial distribution function of the water and sugars around lysozyme was used to monitor the preferential hydration. Analysis of the solvent and sugar distributions around lysozyme was used to investigate the interfacial solvent and sugar structure near the protein surface.
Efficient Isomerization of Glucose to Fructose over Zeolites in Consecutive Reactions in Alcohol and Aqueous Media.

Isomerization reactions of glucose were catalyzed by different types of commercial zeolites in methanol and water in two reaction steps. The most active catalyst was zeolite Y, which was found to be more active than the zeolites beta, ZSM-5, and mordenite. The novel reaction pathway involves glucose isomerization to fructose and subsequent reaction with methanol to form methyl fructoside (step 1), followed by hydrolysis to re-form fructose after water addition (step 2). NMR analysis with (13)C-labeled sugars confirmed this reaction pathway. Conversion of glucose for 1 h at 120 °C with H-USY (Si/Al = 6) gave a remarkable 55% yield of fructose after the second reaction step. A main advantage of applying alcohol media and a catalyst that combines Brønsted and Lewis acid sites is that glucose is isomerized to fructose at low temperatures, while direct conversion to industrially important chemicals like alkyl levulinates is viable at higher temperatures.

General information
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Pages: 5246-5249
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Electrochemical reduction of NiO in a composite electrode

Electrochemical reduction of NiO in a composite electrode along with 8 mol% Y2O3 stabilized zirconia (8YSZ) is studied. Voltage sweeps are performed on cells with a counter electrode made from Pt or the composite of (La0.75Sr0.25)0.95MnO 3 ± δ (LSM25) and 8YSZ, but the composite electrode gives a lower overpotential. Microstructures of NiO with different reduction degrees are shown. Electrochemical impedance spectroscopy is carried out during the reduction process. Electrochemical reduction of NiO may need an induction period. When NiO is reduced at a constant voltage the current initially increases, hereafter a decay is observed. The kinetics of electrochemical reduction of NiO can be described by the Avrami equation. In performed experiments the exponent of the Avrami equation is in the range of 0.5-0.7 and the overall rate constant varies from 1.19 to 7.73 × 10-3 and increases with temperature and in particular with the applied voltage. The maximum reaction rate is obtained when 2-11% NiO is reduced. The increasing resistance in NiO reduction can be exclusively ascribed to one arc in impedance spectra. © 2013 Elsevier B.V.

General information
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Organisations: Department of Energy Conversion and Storage, Fundamental Electrochemistry, Physical and Biophysical Chemistry, Imaging and Structural Analysis
Electrochemistry and in situ scanning tunnelling microscopy of pure and redox-marked DNA- and UNA-based oligonucleotides on Au(111)-electrode surfaces

We have studied adsorption and electrochemical electron transfer of several 13- and 15-base DNA and UNA (unlocked nucleic acids) oligonucleotides (ONs) linked to Au(111)-electrode surfaces via a 50-C6-SH group using cyclic voltammetry (CV) and scanning tunnelling microscopy in aqueous buffer under electrochemical potential control (in situ STM). 2,20,60,200-Terpyridine (terpy) onto which the transition metal ions Fe2+/3+, Os2+/3+ and Ru2+/3+ could be coordinated after UNA monolayer formation was attached to UNA via a flexible linker. The metal centres offer CV probes and in situ STM contrast markers, and the flexible UNA/linker a potential binder for intercalation. CV of pure and mercaptohexanol diluted ON monolayers displayed reductive desorption signals but also, presumably capacitive, signals at higher potentials. Distinct voltammetric signals arise on metal binding. Those from Ru-binding are by far the strongest and in accord with multiple site Ru-attachment. In situ STM disclosed molecular scale features in varying coverage on addition of the metal ions. The Ru-derivatives showed a bias voltage dependent broad maximum in the tunnelling current–overpotential correlation which could be correlated with theoretical frames for condensed matter conductivity of redox molecules. Together the data suggest that Ru-units are bound to both terpy and the UNA–DNA backbone.

General information
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Scopus rating (2015): SJR 1.771 SNIP 1.244 CiteScore 4.45
Web of Science (2015): Indexed yes
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Scopus rating (2014): SJR 1.772 SNIP 1.253 CiteScore 4.29
Web of Science (2014): Indexed yes
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Electrochemistry of Single Metalloprotein and DNA-Based Molecules at Au(111) Electrode Surfaces

We have briefly overviewed recent efforts in the electrochemistry of single transition metal complex, redox metalloprotein, and redox-marked oligonucleotide (ON) molecules. We have particularly studied self-assembled molecular monolayers (SAMs) of several 5′-C6-SH single- (ss) and double-strand (ds) ONs immobilized on Au(111) electrode surfaces via AuS bond formation, using a combination of nucleic acid chemistry, electrochemistry and electrochemically controlled scanning tunnelling microscopy (in situ STM). Ds ONs stabilized by multiply charged cations and locked nucleic acid (LNA) monomers have been primary targets, with a view on stabilizing the ds-ONs and improving voltammetric signals of intercalating electrochemical redox probes. Voltammetric signals of the intercalator anthraquinone monosulfonate (AQMS)
ds-DNA/Au(111) surfaces diluted by mercaptohexanol are significantly sharpened and more robust in the presence than in the absence of [Co(NH3)6]3+. AQMS also displays robust Faradaic voltammetric signals specific to the ds form on binding to similar LNA/Au(111) surfaces, but this signal only evolves after successive voltammetric scanning into negative potential ranges. Triply charged spermidine (Spd) invokes itself a strong voltammetric signal, which is specific to the ds form and fully matched sequences. This signal is of non-Faradaic, capacitive origin but appears in the same potential range as the Faradaic AQMS signal. In situ STM shows that molecular scale structures of the size of Spd-stabilized ds-ONs are densely packed over the Au(111) surface in potential ranges around the capacitive peak potential.
Electrodepositions on Tantalum in Alkali Halide Melts

Surface layers of tantalum metal were electrodeposited on steel from K2TaF7-LiF-NaF-KF melts. With careful control of the oxide contents dense and adherent deposits could be obtained by pulse plating. In NaCl-KCl-NaF-Na2CO3 and NaCl-KCl-Na2CO3 melts carbonate ions seems to be reduced to carbon in a single 4 electron step. By electrolyses at a constant potential of – 1.4 V vs. Pt in a NaCl-KCl-NaF-Na2CO3 melt at 800 °C coherent carbon containing surface layers could be obtained on tantalum substrates, when a CO2 atmosphere was applied.

Aspergillus nidulans Synthesize Insect Juvenile Hormones upon Expression of a Heterologous Regulatory Protein and in Response to Grazing by Drosophila melanogaster Larvae.

Secondary metabolites are known to serve a wide range of specialized functions including communication, developmental control and defense. Genome sequencing of several fungal model species revealed that the majority of predicted secondary metabolite related genes are silent in laboratory strains, indicating that fungal secondary metabolites remain an underexplored resource of bioactive molecules. In this study, we combine heterologous expression of regulatory proteins in Aspergillus nidulans with systematic variation of growth conditions and observe induced synthesis of insect juvenile hormone-III and methyl farnesoate. Both compounds are sesquiterpenes belonging to the juvenile hormone class. Juvenile hormones regulate developmental and metabolic processes in insects and crustaceans, but have not previously been reported as fungal metabolites. We found that feeding by Drosophila melanogaster larvae induced synthesis of juvenile hormone in A. nidulans indicating a possible role of juvenile hormone biosynthesis in affecting fungal-insect antagonisms.
**Cis–Trans Amide Bond Rotamers in β-Peptoids and Peptoids: Evaluation of Stereoelectronic: Effects in Backbone and Side Chains**

Non-natural peptide analogs have significant potential for the development of new materials and pharmacologically active ligands. One such architecture, the β-peptoids (N-alkyl-β-alanines), has found use in a variety of biologically active compounds, but has been sparsely studied with respect to folding propensity. Thus, we here report an investigation of the effect of structural variations on the cis–trans amide bond rotamer equilibria in a selection of monomer model systems. In addition to various side chain effects, which correlated well with previous studies of α-peptoids, we present the synthesis and investigation of cis–trans isomerism in the first examples of peptoids and β-peptoids containing thioamide bonds as well as trifluoroacetylated peptoids and β-peptoids. These systems revealed an increase in the preference for cis-amides as compared to their parent compounds, and thus provide novel strategies for affecting the folding of peptoid constructs. By using NMR spectroscopy, X-ray crystallographic analysis, and density functional theory calculations, we present evidence for the presence of thioamide–aromatic interactions through $C_{sp^2}$H⋯$S_{amide}$ hydrogen bonding, which stabilize certain peptoid conformations.

**General information**

State: Published
Organisations: Department of Chemistry, Organic Chemistry, X-ray Crystallography
Authors: Laursen, J. S. (Intern), Engel-Andreasen, J. (Intern), Fristrup, P. (Intern), Harris, P. (Intern), Olsen, C. A. (Intern)
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- Web of Science (2015): Indexed yes
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- Scopus rating (2014): SJR 6.273 SNIP 2.578 CiteScore 11.92
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- Scopus rating (2011): SJR 5.447 SNIP 2.336 CiteScore 9.94
- ISI indexed (2011): ISI indexed yes
- Web of Science (2011): Indexed yes
- BFI (2010): BFI-level 2
- Scopus rating (2010): SJR 5.076 SNIP 2.132
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
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General information
State: Published
Organisations: Department of Chemistry, Analytical Chemistry, Johannes Kepler Universität Linz, University of Plymouth
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Scopus rating (2016): CiteScore 3.03 SJR 0.943 SNIP 1.039
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.064 SNIP 1.083 CiteScore 3.07
Web of Science (2015): Indexed yes
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Scopus rating (2014): SJR 1.126 SNIP 1.222 CiteScore 3.26
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.229 SNIP 1.282 CiteScore 3.55
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.347 SNIP 1.282 CiteScore 3.51
ISI indexed (2012): ISI indexed yes
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Scopus rating (2011): SJR 1.363 SNIP 1.275 CiteScore 3.47
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.354 SNIP 1.236
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.272 SNIP 1.237
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Scopus rating (2013): SJR 0.269 SNIP 0.613 CiteScore 0.88
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Scopus rating (2012): SJR 0.308 SNIP 0.714 CiteScore 0.98
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ISI indexed (2011): ISI indexed yes
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Scopus rating (2010): SJR 0.275 SNIP 0.56
Web of Science (2010): Indexed yes
Scopus rating (2009): SJR 0.28 SNIP 0.475
Web of Science (2009): Indexed yes
Scopus rating (2008): SJR 0.296 SNIP 0.546
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.237 SNIP 0.592
Scopus rating (2006): SJR 0.261 SNIP 0.481
Scopus rating (2005): SJR 0.198 SNIP 0.529
Exploring the conformational and reactive dynamics of biomolecules in solution using an extended version of the glycine reactive force field

In order to describe possible reaction mechanisms involving amino acids, and the evolution of the protonation state of amino acid side chains in solution, a reactive force field (ReaxFF-based description) for peptide and protein simulations has been developed as an expansion of the previously reported glycine parameters. This expansion consists of adding to the training set more than five hundred molecular systems, including all the amino acids and some short peptide structures, which have been investigated by means of quantum mechanical calculations. The performance of this ReaxFF protein force field on a relatively short time scale (500 ps) is validated by comparison with classical non-reactive simulations and experimental data of well characterized test cases, comprising capped amino acids, peptides, and small proteins, and reaction mechanisms connected to the pharmaceutical sector. A good agreement of ReaxFF predicted conformations and kinetics with reference data is obtained.
Expression, purification and characterization of human Dopamine β-monooxygenase

This thesis deals with expression, purification and characterization of the copper containing enzyme dopamine β-monooxygenase (DBM). DBM is an ascorbate dependent protein that requires Cu in the active site in order to be functional. DBM is made of four domains; An Nterminal DOMON domain, the two catalytic domains called ascorbate dependent type IImonooxygenase domains and a C-terminal dimerization domain. DBM is related to peptidylglycine α-hydroxylating monooxygenase (PHM). They are 28 % identical over approximately 300 amino acids (AA) which corresponds to the catalytic domains. This is, among others, one of the reasons why these proteins are considered to follow the same mechanism. DBM converts dopamine (DA) into Norepinphrine (NE). Both substrate and product functions as neurotransmitters and the levels of these are involved in many different disorders such as depression and hypertension and also the reason why DBM in the past decades has been considered an important therapeutic target. The ambition with this project was to develop a solid and efficient expression system for human DBM (hDBM) and subsequent to characterize it with mass spectrometry (MS) and X-ray crystallography.

hDBM has been successfully expressed in the mammalian HEK293S cells in a stable glycosylated form. The protein has been purified to a very high degree of purity. The purification was done with a FLAG-tag purification followed by a size exclusion step. The protein exists in to active homo-oligomer forms, a dimer and a tetramer. The dimer is held together by two intermolecular disulfide bonds (dsb), while the tetramer consists of two dimers held together by noncovalent interaction. The size and extent of glycosylation and other post translational modifications (PTM) has been investigated in both forms using intact MS analysis and it is concluded that they both contain four oligomannose groups primarily in the GlcNAc2MANN5 form. This means that the enzyme despite the extent of glycosylation is very homogenous. The extent of other PTMs is minimal. The equilibrium between the two oligomer forms is likewise looked into with MS, in regards to pH and ionic strength and it is concluded that the tetramer is stable under the investigated conditions. The stability of the fully glycosylated dimer and tetramer and a partly deglycosylated tetramer was investigated with differential scanning
fluorimetry (DSF). It was found that the tetramer was significantly more stable than the dimer and that to two tetramer forms were equally stable. The effect of ascorbic acid (Asc) and DA on the stability of the protein was also evaluated with DSF, and the conclusion was that the presence of both substrates had a significant effect on the stability of all forms of hDBM. The results from DSF support the result from MS regarding the equilibrium between the two forms. They are not in equilibrium and the presence of DA and Asc do not affect that. Both oligomers were used for crystallization trials and the dimer formed crystals with a 2.9 Å resolution. The structure could however not be solved from molecular replacement (MR) alone and Selenomethionine (Semet) substituted hDBM was hence produced and likewise formed crystals from where the experimental phase could be solved. The first three dimensional (3D) structure of DBM dimer, going from residue 47-596 in each chain, was hereafter manually built. The structure reveals the first structural insights into the DOMON domain and the C-terminal dimerization domain and it shows two different conformations of the catalytic domains. An open conformation, that resembles the structures known from PHM and a closed conformation that brings the two copper sites very close. The closed confirmation has never been observed in PHM and it opens up for a new understanding of how these enzymes functions. This project has contributed with a lot of new and significant knowledge concerning DBM and in addition provided a stable and efficient expression system which is decisive for future characterization of this fascinating protein.

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Extracellular DNA Shields against Aminoglycosides in Pseudomonas aeruginosa Biofilms
Within recent years, it has been established that extracellular DNA is a key constituent of the matrix of microbial biofilms. In addition, it has recently been demonstrated that DNA binds positively charged antimicrobials such as aminoglycosides and antimicrobial peptides. In the present study, we provide evidence that extracellular DNA shields against aminoglycosides in Pseudomonas aeruginosa biofilms. We show that exogenously supplemented DNA integrates into P. aeruginosa biofilms and increases their tolerance toward aminoglycosides. We provide evidence that biofilms formed by a DNA release-deficient P. aeruginosa quorum-sensing mutant are more susceptible to aminoglycoside treatment than wild-type biofilms but become rescued from the detrimental action of aminoglycosides upon supplementation with exogenous DNA. Furthermore, we demonstrate that exposure to lysed polymorphonuclear leukocytes, which are thought to be a source of extracellular DNA at sites of infections, increases the tolerance of P. aeruginosa biofilms toward aminoglycosides. Although biofilm-associated aminoglycoside tolerance recently has been linked to extracellular DNA-mediated activation of the pmr genes, we demonstrate that the aminoglycoside tolerance mediated by the presence of extracellular DNA is not caused by activation of the pmr genes in our P. aeruginosa biofilms but rather by a protective shield effect of the extracellular DNA.

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry, University of Copenhagen, Copenhagen University Hospital
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Publication information
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Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
Field-free molecular orientation induced by single-cycle THz pulses: the role of resonance and quantum interference

We consider the rotational excitation of molecules induced by asymmetric ("half-cycle") as well as symmetric single-cycle THz pulses, leading to field-free time-dependent orientation. We show that the basic excitation mechanisms are very similar for the two types of pulses; i.e., the frequency distributions of the pulses at the rotational resonance frequencies play an important role. Furthermore, we investigate the interference between multiple rotational excitation pathways following prealignment with a nonresonant 800-nm femtosecond pulse. It is shown that such interference can lead to an enhancement of the orientation of the linear HCN molecule by a factor close to 2.

General information
State: Published
Organisations: Department of Chemistry, Physical and Biophysical Chemistry
Authors: Shu, C. (Intern), Henriksen, N. E. (Intern)
Number of pages: 6
Pages: Paper 013408
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Main Research Area: Technical/natural sciences

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Journal: Physical Review A
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BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
Scopus rating (2016): CiteScore 2.25 SJR 1.281 SNIP 0.852
Web of Science (2016): Indexed yes
Scopus rating (2015): SJR 1.451 SNIP 0.903 CiteScore 2.06
Web of Science (2015): Indexed yes
Scopus rating (2014): SJR 2.121 SNIP 1.146 CiteScore 2.46
Web of Science (2014): Indexed yes
Scopus rating (2013): SJR 2.317 SNIP 1.179 CiteScore 2.86
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Scopus rating (2012): SJR 2.515 SNIP 1.239 CiteScore 2.81
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
Scopus rating (2011): SJR 2.31 SNIP 1.261 CiteScore 2.79
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
Scopus rating (2010): SJR 2.403 SNIP 1.22
Web of Science (2010): Indexed yes
Scopus rating (2009): SJR 2.475 SNIP 1.305
Web of Science (2009): Indexed yes
Scopus rating (2008): SJR 2.559 SNIP 1.241
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 2.618 SNIP 1.259
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 2.342 SNIP 1.257
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 2.017 SNIP 1.286
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 2.168 SNIP 1.1
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 2.05 SNIP 1.078
Web of Science (2003): Indexed yes
Filming the Birth of Molecules and Accompanying Solvent Rearrangement

Molecules are often born with high energy and large-amplitude vibrations. In solution, a newly formed molecule cools down by transferring energy to the surrounding solvent molecules. The progression of the molecular and solute–solvent cage structure during this fundamental process has been elusive, and spectroscopic data generally do not provide such structural information. Here, we use picosecond X-ray liquidography (solution scattering) to visualize time-dependent structural changes associated with the vibrational relaxation of I₂ molecules in two different solvents, CCl₄ and cyclohexane. The birth and vibrational relaxation of I₂ molecules and the associated rearrangement of solvent molecules are mapped out in the form of a temporally varying interatomic distance distribution. The I–I distance increases up to ∼4 Å and returns to the equilibrium distance (2.67 Å) in the ground state, and the first solvation cage expands by ∼1.5 Å along the I–I axis and then shrinks back accompanying the structural change of the I₂ molecule.
Formation of carboxy- and amide-terminated alkyl monolayers on silicon(111) investigated by ATR-FTIR, XPS, and X-ray scattering: Construction of photoswitchable surfaces

We have prepared high-quality, densely packed, self-assembled monolayers (SAMs) of carboxy-terminated alkyl chains on Si(111). The samples were made by thermal grafting of methyl undec-10-enoate under an inert atmosphere and subsequent cleavage of the ester functionality to disclose the carboxylic acid end-group. X-ray photoelectron spectroscopy (XPS) and grazing incidence X-ray diffraction (GIXD) indicate a surface coverage of about 50% of the initially H-terminated
sites. In agreement, GIXD implies a rectangular unit mesh of 6.65 and 7.68 Å side lengths, containing two molecules in a regular zigzag-like substitution pattern for the ester- and carboxy-terminated monolayer. Hydrolysis of the remaining H-Si(111) bonds at the surface furnished HO-Si(111) groups according to XPS and attenuated total reflection Fourier-transform infrared spectroscopy (ATR-FTIR) studies. The amide-terminated alkyl SAM on Si(111) assembled in a 2-(6-chloro-1H-benzotriazol-1-yl)-1,1,3,3-tetramethyluronium hexafluorophosphate (HCTU)-mediated one-pot coupling reaction under an inert atmosphere, whereby the active ester forms in situ prior to the reaction with an amino-functionalized photoswitchable fulgimide. ATR-FTIR and XPS studies of the fulgimide samples revealed closely covered amide-terminated SAMs. Reversible photoswitching of the headgroup was read out by applying XPS, ATR-FTIR, and difference absorption spectra in the mid-IR. In XPS, we observed a reversible breathing of the amide/imide C1s and N1s signals of the fulgimide. The results demonstrate the general suitability of HCTU as a reagent for amide couplings to carboxy-terminated alkyl SAMs and the on-chip functionalization toward photoswitchable Si(111) surfaces. © 2013 American Chemical Society.
Frictional forces between hydrophilic and hydrophobic particle coated nanostructured surfaces

Friction forces have long been associated with the famous Amontons' rule that states that the friction force is linearly dependent on the applied normal load, with the proportionality constant being known as the friction coefficient. Amontons' rule is however purely phenomenological and does not in itself provide any information on why the friction coefficient is different for different material combinations. In this study, friction forces between a colloidal probe and nanostructured particle coated surfaces in an aqueous environment exhibiting different roughness length scales were measured by utilizing the atomic force microscope (AFM). The chemistry of the surfaces and the probe was varied between hydrophilic silica and hydrophobized silica. For hydrophilic silica surfaces, the friction coefficient was significantly higher for the particle coated surfaces than on the flat reference surface. All the particle coated surfaces exhibited similar friction coefficients, from which it may be concluded that the surface geometry, and not the roughness amplitude per se, influenced the measured friction. During measurements with hydrophobic surfaces, strong adhesive forces related to the formation of a bridging air cavity were evident from both normal force and friction force measurements. In contrast to the frictional forces between the hydrophilic surfaces, the friction coefficient for hydrophobic surfaces was found to depend on the surface structure and we believe that this dependence is related to the restricted movement of the three-phase line of the bridging air cavity. For measurements using a hydrophobic surface and a hydrophilic probe, the friction coefficient was significantly smaller compared to the two homogeneous systems. A layer of air or air bubbles on the hydrophobic surface working as a lubricating layer is a possible mechanism behind this observation.
Further elucidation of the Grignard-addition reaction

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry
Authors: Christensen, S. H. (Intern), Holm, T. (Intern), Madsen, R. (Intern)
Publication date: 2013
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Web of Science (2018): Indexed yes
Web of Science (2017): Indexed Yes
Scopus rating (2014): SJR 0.101 SNIP 0.013
Web of Science (2014): Indexed yes
Scopus rating (2013): SJR 0.101 SNIP 0.003
Web of Science (2013): Indexed yes
Scopus rating (2012): SJR 0.1 SNIP 0
Scopus rating (2011): SJR 0.101 SNIP 0
Web of Science (2011): Indexed yes
Scopus rating (2010): SJR 0.101 SNIP 0
Scopus rating (2009): SJR 0.101 SNIP 0
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 0.101 SNIP 0
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.101 SNIP 0
Scopus rating (2006): SJR 0.101
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.101
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 0.104 SNIP 0.028
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 0.111 SNIP 0.008
Scopus rating (2002): SJR 0.115 SNIP 0.046
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 0.111 SNIP 0.038
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 0.111
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Publication: Research - peer-review » Conference abstract in journal – Annual report year: 2013

Graphene Paper Doped with Chemically Compatible Prussian Blue Nanoparticles as Nanohybrid Electrocatalyst
Along with reduced graphene oxide (RGO), water soluble Prussian blue nanoparticles (PBNPs, around 6 nm) are synthesized and broadly characterized. These two types of highly stable, low-cost and chemically compatible nanomaterials are exploited as building ingredients to prepare electrically enhanced and functionally endorsed nanohybrid electrocatalysts, which are further transformed into free-standing graphene papers. PBNP\textquoteright s doped graphene papers show highly efficient electrocatalysis towards reduction of hydrogen peroxide and can be used alone as flexible chemical
sensors for potential applications in detection of hydrogen peroxide or/and other organic peroxides. The as-prepared PBNPs–RGO papers are further capable of biocompatible accommodation of enzymes for development of free-standing enzyme based biosensors. In this regard, glucose oxidase is used as an example for electrocatalytic oxidation and detection of glucose. The present work demonstrates a facile and highly reproducible way to construct free-standing and flexible graphene paper doped with electroactive catalyst. Thanks to high stability, low-cost and efficient electrocatalytic characteristics, this kind of nanohybrid material has potential to be produced on a large scale, and offers a broad range of possible applications, particularly in the fabrication of flexible sensing devices and as a platform for electrocatalytic energy conversion.

General information
State: Published
Organisations: Department of Chemistry, NanoChemistry
Authors: Zhu, N. (Intern), Han, S. (Intern), Gan, S. (Intern), Ulstrup, J. (Intern), Chi, Q. (Intern)
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Main Research Area: Technical/natural sciences

Publication information
Journal: Advanced Functional Materials
Volume: 23
Issue number: 42
ISSN (Print): 1616-301X
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 11.56
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): CiteScore 11.93
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): CiteScore 11.32
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): CiteScore 10.6
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): CiteScore 10.41
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): CiteScore 9.47
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 2
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 2
Web of Science (2008): Indexed yes
Web of Science (2007): Indexed yes
Original language: English
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10.1002/adfm.201300605
Source: dtu
Source-ID: n:oat:DTIC-ART:wiley/425294462::33985
Publication: Research - peer-review › Journal article – Annual report year: 2013
Heterometallic [AgFe$_3$S$_4$] ferredoxin variants: synthesis, characterization, and the first crystal structure of an engineered heterometallic iron–sulfur protein

Heterometallic [AgFe$_3$S$_4$] iron–sulfur clusters assembled in wild-type Pyrococcus furiosus ferredoxin and two variants, D14C and D14H, are characterized. The crystal structure of the [AgFe$_3$S$_4$] D14C variant shows that the silver(I) ion is indeed part of the cluster and is coordinated to the thiolate group of residue 14. Cyclic voltammetry shows one redox pair with a reduction potential of +220 mV versus the standard hydrogen electrode which is assigned to the [AgFe$_3$S$_4$]$_2^+/+$ couple. The oxidized form of the [AgFe$_3$S$_4$] D14C variant is stable in the presence of dioxygen, whereas the oxidized forms of the [AgFe$_3$S$_4$] wild type and D14H variants convert to the [Fe$_3$S$_4$] ferredoxin form. The monovalent d 10 silver(I) ion stabilizes the [Fe$_3$S$_4$]+/0 cluster fragment, as opposed to divalent d 10 metal ions, resulting in more than 0.4 V difference in reduction potentials between the silver(I) and, e.g., zinc(II) heterometallic [MFe$_3$S$_4$] ferredoxins. The trend in reduction potentials for the variants containing the [AgFe$_3$S$_4$] cluster is wild type ≤ D14C < D14H and shows the same trend as reported for the variants containing the [Fe$_3$S$_4$] cluster, but is different from the D14C < D14H < wild type trend reported for the [Fe$_4$S$_4$] ferredoxin. The similarity in the reduction potential trend for the variants containing the heterometallic [AgFe$_3$S$_4$] cluster and the [Fe$_3$S$_4$] cluster can be rationalized in terms of the electrostatic influence of the residue 14 side chains, rather than the dissociation constant of this residue, as is the case for [Fe$_4$S$_4$] ferredoxins. The trends in reduction potentials are in line with there being no electronic coupling between the silver(I) ion and the Fe$_3$S$_4$ fragment.

General information
State: Published
Organisations: Department of Chemistry, Metalloprotein Chemistry and Engineering, Delft University of Technology
Authors: Martic, M. (Intern), Simon, I. N. (Intern), Haahr, L. T. (Intern), Hagen, W. R. (Ekstern), Christensen, H. E. M. (Intern)
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Publication date: 2013
Main Research Area: Technical/natural sciences

Publication information
Journal: Journal of Biological Inorganic Chemistry
Volume: 18
Issue number: 2
ISSN (Print): 0949-8257
Ratings:
BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 1
Scopus rating (2016): SJR 0.857 SNIP 0.761 CiteScore 2.4
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.869 SNIP 0.778 CiteScore 2.33
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.963 SNIP 0.938 CiteScore 2.65
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 1.092 SNIP 1.058 CiteScore 3.16
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 1.175 SNIP 0.982 CiteScore 3.03
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 1.263 SNIP 0.983 CiteScore 3.18
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 1.215 SNIP 0.936
BFI (2009): BFI-level 2
High purity $\text{H}_2/\text{H}_2\text{O}/\text{Ni}/\text{SZ}$ electrodes at 500º C

The performance of SOFC (solid oxide fuel cell) anodes is influenced negatively by impurities. In the present study segregation of impurities is minimized by using high purity materials at relatively low temperatures to prevent fast segregation. Ni point electrodes on polished single crystals of stabilized zirconia (SZ) with 10, 13 and 18 mol% yttria and one with 6 mol% scandia plus 4 mol% yttria were studied at open circuit voltage at 400-500 ºC in mixtures of $\text{H}_2/\text{H}_2\text{O}$ over 46 days. The polarization resistances ($R_p$) for all samples increased significantly during the first 10-20 days at 500 ºC. No effect of the electrolyte composition on $R_p$ was found. Surface sensitive techniques were used to analyze the composition of the nickel and the electrolytes before and after the electrochemical experiment. Impurities were found to segregate to the surfaces/interfaces, and they are believed to impede the electrode processes and hence to cause the increase in polarization resistance. © 2013 Elsevier B.V.

General information
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Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry, Imaging and Structural Analysis, Fundamental Electrochemistry, Department of Physics, Experimental Surface and Nanomaterials Physics, Physical and Biophysical Chemistry, Department of Chemistry
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Publication date: 2013
Main Research Area: Technical/natural sciences
High-resolution rovibrational analysis of CH281BrF in the range 920–980cm−1

The high-resolution infrared spectrum of CH281BrF has been studied in part of the atmospheric window between 920 and 980cm−1, the region characterized by the v9 and v5+v6 absorptions. The v9 emerges as a pseudo a-type band, with selection rule ΔKa=ΔKc=0, ±2, and v5+v6 exhibits a predominant a-type structure. The interactions connecting these levels and the dark 3v6 state have been explored. The anomalous v9 transitions have been ascribed to Coriolis interaction with v4. The analysis yields a set of accurate upper-state parameters for v9 and v5+v6. Spectroscopic information on 3v6
has been also obtained.

**General information**

State: Published
Organisations: Department of Chemistry, Universitá Ca' Foscari Venezia, Georg-August-Universität Göttingen
Authors: Visinoni, R. (Ekstern), Baldacci, A. (Ekstern), Stoppa, P. (Ekstern), Kollipost, F. (Ekstern), Larsen, R. W. (Intern)
Pages: 16-22
Publication date: 2013
Main Research Area: Technical/natural sciences

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Ratings:
- BFI (2018): BFI-level 1
- Web of Science (2018): Indexed yes
- BFI (2017): BFI-level 1
- Web of Science (2017): Indexed Yes
- BFI (2016): BFI-level 1
- Scopus rating (2016): CiteScore 1.71 SJR 0.726 SNIP 0.721
- BFI (2015): BFI-level 1
- Scopus rating (2015): SJR 0.733 SNIP 0.747 CiteScore 1.83
- BFI (2014): BFI-level 1
- Scopus rating (2014): SJR 0.757 SNIP 0.773 CiteScore 1.83
- BFI (2013): BFI-level 1
- Scopus rating (2013): SJR 0.856 SNIP 0.844 CiteScore 2.07
- ISI indexed (2013): ISI indexed yes
- Web of Science (2013): Indexed yes
- BFI (2012): BFI-level 1
- Scopus rating (2012): SJR 1.101 SNIP 0.916 CiteScore 2.2
- ISI indexed (2012): ISI indexed yes
- Web of Science (2012): Indexed yes
- BFI (2011): BFI-level 1
- Scopus rating (2011): SJR 1.156 SNIP 1.013 CiteScore 2.38
- ISI indexed (2011): ISI indexed yes
- Web of Science (2011): Indexed yes
- BFI (2010): BFI-level 1
- Scopus rating (2010): SJR 1.207 SNIP 0.94
- Web of Science (2010): Indexed yes
- BFI (2009): BFI-level 1
- Scopus rating (2009): SJR 1.234 SNIP 0.972
- Web of Science (2009): Indexed yes
- BFI (2008): BFI-level 1
- Scopus rating (2008): SJR 1.296 SNIP 0.937
- Web of Science (2008): Indexed yes
- Scopus rating (2007): SJR 1.43 SNIP 1.001
- Web of Science (2007): Indexed yes
- Scopus rating (2006): SJR 1.483 SNIP 1.107
- Web of Science (2006): Indexed yes
- Scopus rating (2005): SJR 1.503 SNIP 1.086
- Web of Science (2005): Indexed yes
- Scopus rating (2004): SJR 1.512 SNIP 1.129
- Web of Science (2004): Indexed yes
- Scopus rating (2003): SJR 1.556 SNIP 1.156
- Web of Science (2003): Indexed yes
Hyaluronan and phospholipid association in biolubrication

It is becoming increasingly clear that the outstanding lubrication of synovial joints is achieved by a sophisticated hierarchical structure of cartilage combined with synergistic actions of surface-active components present in the synovial fluid. In this work we focus on the association of two components of the synovial fluid, hyaluronan and dipalmitoyl phosphatidyl choline (DPPC), in bulk solution and at interfaces. We demonstrate that hyaluronan associates with DPPC vesicles and adsorbs to supported DPPC bilayers. The association structures formed at the interface are sufficiently stable to allow sequential adsorption of DPPC and hyaluronan, whereby promoting the formation of thick composite layers of these two components. The lubricating ability of such composite layers was probed by the AFM colloidal probe technique and found to be very favorable with low friction coefficients and high load bearing capacity. With DPPC as the last adsorbed component, a friction coefficient of 0.01 was found up to pressures significantly above what is encountered in healthy synovial joints. Hyaluronan as the last added component increases the friction coefficient to 0.03 and decreases the load bearing capacity somewhat (but still above what is needed in the synovial joint). Our data demonstrate that self-assembly structures formed by hyaluronan and phospholipids at interfaces are efficient aqueous lubricants, and it seems plausible that such self-assembly structures contribute to the exceptional lubrication of synovial joints. © 2013 American Chemical Society.

General information

State: Published
Organisations: Department of Chemistry, KTH - Royal Institute of Technology, SP Technical Research Institute of Sweden
Authors: Wang, M. (Ekstern), Liu, C. (Ekstern), Thormann, E. (Intern), Dedinaite, A. (Ekstern)
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Publication date: 2013
Main Research Area: Technical/natural sciences

Publication information
Journal: Biomacromolecules
Volume: 14
Issue number: 12
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Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 5.74 SJR 1.973 SNIP 1.334
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 2.134 SNIP 1.449 CiteScore 6.05
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.207 SNIP 1.652 CiteScore 6.38
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 2.085 SNIP 1.617 CiteScore 6.07
Hydrophobic Surfaces: Topography Effects on Wetting by Supercooled Water and Freezing Delay

Hydrophobicity, and in particular superhydrophobicity, has been extensively considered to promote ice-phobicity. Dynamic contact angle measurements above 0 °C have been widely used to evaluate the water repellency. However, it is the wetting properties of supercooled water at subzero temperatures and the derived work of adhesion that are important for applications dealing with icing. In this work we address this issue by determining the temperature-dependent dynamic contact angle of microliter-sized water droplets on a smooth hydrophobic and a superhydrophobic surface with similar surface chemistry. The data highlight how the work of adhesion of water in the temperature interval from about 25 °C to below −10 °C is affected by surface topography. A marked decrease in contact angle on the superhydrophobic surface is observed with decreasing temperature, and we attribute this to condensation below the dew point. In contrast, no significant wetting transition is observed on the smooth hydrophobic surface. The freezing temperature and the freezing delay time were determined for water droplets resting on a range of surfaces with similar chemistry but different topography, including smooth and rough surfaces in either the Wenzel or the Cassie–Baxter state as characterized by water contact angle measurements at room temperature. We find that the water freezing delay time is not significantly
affected by the surface topography and discuss this finding within the classical theory of heterogeneous nucleation.

**General information**
State: Published
Organisations: Department of Chemistry, KTH - Royal Institute of Technology, SP Technical Research Institute of Sweden
Authors: Heydari, G. (Ekstern), Thormann, E. (Intern), Järn, M. (Ekstern), Tyrode, E. (Ekstern), Claesson, P. (Forskerdatabase)
Pages: 21752-21762
Publication date: 2013
Main Research Area: Technical/natural sciences

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BFI (2018): BFI-level 1
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 4.48 SJR 1.948 SNIP 1.181
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.917 SNIP 1.268 CiteScore 4.68
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.027 SNIP 1.448 CiteScore 5.08
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 2.134 SNIP 1.439 CiteScore 5.14
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.514 SNIP 1.46 CiteScore 4.98
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.32 SNIP 1.457 CiteScore 4.92
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 2.438 SNIP 1.356
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 2.128 SNIP 1.417
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.856 SNIP 1.033
Web of Science (2008): Indexed yes
Web of Science (2007): Indexed yes
Web of Science (2006): Indexed yes
Web of Science (2005): Indexed yes
Web of Science (2004): Indexed yes
Web of Science (2003): Indexed yes
Identification of Five Structurally Unrelated Quorum-Sensing Inhibitors of Pseudomonas aeruginosa from a Natural-Derivative Database

Bacteria communicate by means of small signal molecules in a process termed quorum sensing (QS). QS enables bacteria to organize their activities at the population level, including the coordinated secretion of virulence factors. Certain small-molecule compounds, known as quorum-sensing inhibitors (QSIs), have been shown to effectively block QS and subsequently attenuate the virulence of Pseudomonas aeruginosa, as well as increasing its susceptibility to both antibiotics and the immune system. In this study, a structure-based virtual screening (SB-VS) approach was used for the discovery of novel QSI candidates. Three-dimensional structures of 3,040 natural compounds and their derivatives were obtained, after which molecular docking was performed using the QS receptor LasR as a target. Based on docking scores and molecular masses, 22 compounds were purchased to determine their efficacies as quorum-sensing inhibitors. Using a live reporter assay for quorum sensing, 5 compounds were found to be able to inhibit QS-regulated gene expression in P. aeruginosa in a dose-dependent manner. The most promising compound, G1, was evaluated by isobaric tag for relative and absolute quantitation (iTRAQ)-based proteomic analysis, and it was found to significantly affect the abundance of 46 proteins (19 were upregulated; 27 were downregulated) in P. aeruginosa PAO1. It specifically reduced the expression of several quorum-sensing-regulated virulence factors, such as protease IV, chitinase, and pyoverdine synthetases. G1 was also able to reduce extracellular DNA release and inhibited the secretion of the virulence factor, elastase, whose expression is regulated by LasR. These results demonstrate the utility of SB-VS for the discovery of target-specific QSIs.
During our search for new natural products from the marine environment, we discovered a wide range of cyclic peptides from a marine Photobacterium, closely related to P. halotolerans. The chemical fingerprint of the bacterium showed primarily non-ribosomal peptide synthetase (NRPS)-like compounds, including the known pyrrothine antibiotic holomycin and a wide range of peptides, from diketopiperazines to cyclodepsipeptides of 500–900 Da. Purification of components from the pellet fraction led to the isolation and structure elucidation of four new cyclodepsipeptides, ngercheumicin F, G, H, and I. The ngercheumicins interfered with expression of virulence genes known to be controlled by the agr quorum sensing system of Staphylococcus aureus, although to a lesser extent than the previously described solonamides from the same strain of Photobacterium.

**General information**

State: Published

Organisations: Department of Chemistry, Organic Chemistry, Department of Systems Biology, Natural Product Chemistry, Bacterial Ecophysiology and Biotechnology, University of Copenhagen

Authors: Kjærulff, L. (Intern), Nielsen, A. (Ekstern), Månsson, M. (Intern), Gram, L. (Intern), Larsen, T. O. (Intern), Ingmer, H. (Ekstern), Gotfredsen, C. H. (Intern)
Identification of LasR Ligands through a Virtual Screening Approach

With the widespread occurrence of bacterial resistance to antibiotics, the development of new strategies beyond conventional treatments is a pursuit taken by public health institutions worldwide. LasR, a transcription factor that controls quorum sensing in Pseudomonas aeruginosa, has emerged as an attractive therapeutic target for the next generation of antimicrobial agents. In the present study, a virtual screening workflow combining pharmacophore- and structure-based approaches was used to identify new LasR ligands. Five novel inducers and three inhibitors of LasR activity were validated experimentally by use of a cell-based assay. Interestingly, these compounds are molecularly distinct from the
native signal molecule, N-3-oxododecanoyl-L-homoserine lactone (OHN), and may serve as lead structures for the design of new drugs. The binding modes of these compounds to the OHN binding site in LasR were predicted and used to identify the key interactions that contribute to the induction and inhibition of LasR activity.

**General information**

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Organisations: Organic Chemistry, Department of Chemistry, Center for Biological Sequence Analysis, Department of Systems Biology, University of Copenhagen, Technical University of Denmark
Pages: 157-163
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Web of Science (2017): Indexed Yes
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Scopus rating (2016): SJR 1.13 SNIP 0.906 CiteScore 3.11
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.148 SNIP 0.905 CiteScore 3
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.11 SNIP 0.907 CiteScore 2.83
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.142 SNIP 0.845 CiteScore 2.93
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.125 SNIP 0.814 CiteScore 2.87
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.263 SNIP 0.928 CiteScore 3.24
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.264 SNIP 0.923
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.188 SNIP 0.89
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.272 SNIP 0.905
Scopus rating (2007): SJR 0.991 SNIP 1.127
Web of Science (2007): Indexed yes
Scopus rating (2006): SNIP 0.9
Scopus rating (2005): SNIP 0.85
Scopus rating (2004): SNIP 0.847
Scopus rating (2003): SNIP 0.911
Scopus rating (2002): SNIP 0.83
Scopus rating (2001): SNIP 0.628
Improved controlled atmosphere high temperature scanning probe microscope

To locally access electrochemical active surfaces and interfaces in operando at the sub-micron scale at high temperatures in a reactive gas atmosphere is of great importance to understand the basic mechanisms in new functional materials, for instance, for energy technologies, such as solid oxide fuel cells and electrolyzer cells. Here, we report on advanced improvements of our original controlled atmosphere high temperature scanning probe microscope, CAHT-SPM. The new microscope can employ a broad range of the scanning probe techniques including tapping mode, scanning tunneling microscopy, scanning tunneling spectroscopy, conductive atomic force microscopy, and Kelvin probe force microscopy. The temperature of the sample can be as high as 850 °C. Both reducing and oxidizing gases such as oxygen, hydrogen, and nitrogen can be added in the sample chamber and the oxygen partial pressure (pO₂) is monitored by an oxygen sensor. We present here some examples of its capabilities demonstrated by high temperature topography with simultaneously ac electrical conductance measurements during atmosphere changes, electrochemical impedance spectroscopy at various temperatures, and measurements of the surface potential. The improved CAHT-SPM, therefore, holds a great potential for local sub-micron analysis of high-temperature and gas induced changes of a wide range of materials.

General information
State: Published
Organisations: Department of Energy Conversion and Storage, Imaging and Structural Analysis, Department of Chemistry, Physical and Biophysical Chemistry, Fundamental Electrochemistry
Authors: Hansen, K. V. (Intern), Wu, Y. (Intern), Jacobsen, T. (Intern), Mogensen, M. B. (Intern), Kuhn, L. T. (Intern)
Number of pages: 7
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Publication date: 2013
Main Research Area: Technical/natural sciences

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Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.2 SJR 0.585 SNIP 0.855
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.562 SNIP 0.824 CiteScore 1.11
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.922 SNIP 1.211 CiteScore 1.45
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.898 SNIP 1.117 CiteScore 1.28
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.012 SNIP 1.267 CiteScore 1.45
ISI indexed (2012): ISI indexed yes
The present invention relates to screening of one-bead-one-compound (OBOC) combinatorial libraries which is useful for the discovery of compounds displaying molecular interactions with a biological or a physicochemical system, such as substrates and inhibitors of enzymes and the like. The invention provides a method for screening a library of compounds for their interaction with a physico-chemical or biological system and a corresponding kit for performing the method of screening a one-bead-one-compound library of compounds.

In-bead screening
The present invention relates to screening of one-bead-one-compound (OBOC) combinatorial libraries which is useful for the discovery of compounds displaying molecular interactions with a biological or a physicochemical system, such as substrates and inhibitors of enzymes and the like. The invention provides a method for screening a library of compounds for their interaction with a physico-chemical or biological system and a corresponding kit for performing the method of screening a one-bead-one-compound library of compounds.

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry
Authors: Nielsen, T. E. (Intern), Qvortrup, K. (Intern)
Publication date: 2013

Publication information
IPC: G01N33/50
Patent number: WO2013057188
Date: 18/10/2012
Original language: English
In-situ SEM microchip setup for electrochemical experiments with water based solutions

Studying electrochemical (EC) processes with electron microscopes offers the possibility of achieving much higher resolution imaging of nanoscale processes in real time than with optical microscopes. We have developed a vacuum sealed liquid sample electrochemical cell with electron transparent windows, microelectrodes and an electrochemical reference electrode. The system, called the EC-SEM Cell, is used to study electrochemical reactions in liquid with a standard scanning electron microscope (SEM). The central component is a microfabricated chip with a thin (50nm) Si-rich silicon nitride (SiNx) window with lithographically defined platinum microelectrodes. We show here the design principles of the EC-SEM system, its detailed construction and how it has been used to perform a range of EC experiments, two of which are presented here. It is shown that the EC-SEM Cell can survive extended in-situ EC experiments. Before the EC experiments we characterized the beam current being deposited in the liquid as this will affect the experiments. The first EC experiment shows the influence of the electron-beam (e-beam) on a nickel solution by inducing electroless nickel deposition on the window when increasing the current density from the e-beam. The second experiment shows electrolysis in EC-SEM Cell, induced by the built-in electrodes.
This work describes an integration between chemistry, molecular biophysics, physiology, sequence evolution and bioinformatics to better understand the evolution of mammalian myoglobins (Mb) in terms of their primary biochemical function (i.e., O2 binding) and their thermodynamic stability (i.e., folding free energy). First, we merge a large set of previously reported thermochemical data for Mb mutants with a physiological model of O2 delivery in the skeletal muscle cells to quantify the functional proficiency of Mb mutants under various physiological conditions. We find that O2-storage and –transport are distinct functions which depend on O2 partial pressure and conclude that conserved residues in wild type (WT) Mb were fixated under a selection pressure of low $P_{O2}$.

Second, we present an integrated model of convective O2-transport and O2-affinity of mutant Mb to quantify the impacts of mutations in Mb on the aerobic dive limits (ADL) of Weddell seals (Leptonychotes weddellii). We show that wild-type Mb traits are only superior under specific physiological conditions that critically prolong the ADL, action radius, and fitness of the seals. Third, we deal with the observation of higher folding stabilities (i.e., $\Delta G_{\text{folding}}$) of cetacean Mbs compared to their terrestrial counterparts. Using ancestral sequence reconstruction, maximum likelihood and Bayesian tests to describe the evolution of cetacean Mbs, and experimentally calibrated computation of stability effects of mutations (i.e., $\Delta\Delta G_{\text{folding}}$), we observe accelerated evolution in cetaceans and identify seven positively selected sites in Mb. We show that these sites contribute to Mb stabilization by favoring hydrophobic folding, structural integrity, and intra-helical hydrogen bonds. Finally, we ask a fundamental question that how a general protein phenotype such as folding stability, that was shown as an example to be positively selected in cetacean Mbs in the iv third part of this thesis, affects the rate of protein evolution. Using a model that combines explicit evolution of Mb sequences, folding stability, and application of maximum likelihood (ML) estimation of evolution rate (ER), we find that ER predicted by ML methods is highly correlated with ER from simulations using the explicit sequence information by counting the number of synonymous and nonsynonymous mutations fixed in the population. We show that this agreement is strongest in the regime of high stability where proteins are mostly evolving neutrally. In the unstable regime where protein evolution is dominated by selection for stabilizing mutations we detect a weak yet significant positive selection for specific residues in the sequences from simulations of the order of $dN/dS \approx 1.5$. Overall, this thesis provides one of the first examples in the study of evolution of function and thermodynamic stability in a mammalian protein with implications for fitness. We quantify and highlight the biological relevance for the selection of a higher concentration of Mb in the skeletal muscle of marine mammals and provide an explanation for the increase in folding stability of Mb. Moreover, this thesis provides number of theoretical findings directly testable with future experimental studies regarding the function, physiology and thermodynamic stability of mammalian Mbs.
Inverse Problems in Geosciences: Modelling the Rock Properties of an Oil Reservoir

Even the most optimistic forecasts predict that Danish oil production will decrease by 80% in the period between 2006 and 2040, and only a strong innovative technological effort can change that. Due to the geological structures of the subsurface in the Danish part of the North Sea, Denmark is currently missing out on approximately 70% of the oil, which is left behind, trapped in unreachable parts of the reservoirs.

An increase in the oil recovery rate can be achieved by better planning and optimisation of oil production. Both require an improved description of the rock properties of the subsurface of the reservoirs. Hence the focus of this work has been on acquiring models of spatial parameters describing rock properties of the subsurface using geostatistical a priori knowledge and available geophysical data. Such models are solutions to often severely under-determined, inverse problems.

The focus of the study has been on the computational aspects of inferring such models. Reservoir modelling is a large-scale problem with great computational complexity and the work should be seen as a first part of a foundation for one day, when the computational resources are available, being able to handle the large scale problems of the petroleum industry. But for now most of the study is based on simplified and idealised models.

We have proposed a method for efficient and accurate interpolation of rock properties from seismic data. It is based on a recently published paper on interpolation of rock properties that breaks with the dominating influence of spatial coordinates in traditional interpolation methods. The thesis contains work involving a test case study of the method demonstrating how the interpolation in attribute space ensures the geological structures of the computed models and how the method can be further improved by an orthogonal transformation of the attribute space.

We have formulated a closed form expression of an a priori probability density function that quantifies the statistical probability of models describing the rock properties of a reservoir. This can be used to evaluate the probability that a model adhere to prior knowledge by having specific multiple-point statistics, for instance, learned from a training image. Existing methods efficiently sample an a priori probability density function to create a set of acceptable models; but they cannot evaluate the probability of a model.

We have developed and implemented the Frequency Matching method that uses the closed form expression of the a priori probability density function to formulate an inverse problem and compute the maximum a posteriori solution to it. Other methods for computing models that simultaneously fit data observations and honour a priori knowledge are not capable of computing the maximum a posteriori solution. Instead they either sample the posterior probability density function or they sample the a priori probability density function to optimise the likelihood function.

This thesis consists of a summary report and seven research papers submitted, reviewed and/or published in the period 2010 - 2013.

General information
State: Published
Organisations: Center for Energy Resources Engineering, Department of Applied Mathematics and Computer Science, Scientific Computing, Department of Chemistry
Authors: Lange, K. (Intern), Mosegaard, K. (Intern), Hansen, P. C. (Intern), Stenby, E. H. (Intern)
Number of pages: 248
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Publication information
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In vitro growth of four individual human gut bacteria on oligosaccharides produced by chemoenzymatic synthesis.

The present study aimed at examining oligosaccharides (OS) for potential stimulation of probiotic bacteria. Nineteen structurally well-defined candidate OS covering groups of β-glucosides, α-glucosides and α-galactosides with degree of
polymerization 2-4 were prepared in >100 mg amounts by chemoenzymatic synthesis (i.e. reverse phosphorolysis or transglycosylation). Fourteen of the OS are not naturally occurring and five (β-d-glucosyl-fructose, β-d-glucosyl-xylitol, α-glucosyl-(1,4)-d-mannose, α-glucosyl-(1,4)-d-xyllose; α-glucosyl-(1,4)-l-fucose) have recently been synthesized for the first time. These OS have not been previously tested for effects of bacterial growth and here the ability of all 19 OS to support growth of four gastrointestinal bacteria: three probiotic bacteria Bifidobacterium lactis, Bifidobacterium longum, and Lactobacillus acidophilus, and one commensal bacterium, Bacteroides vulgatus has been evaluated in monocultures. The disaccharides β-d-glucosyl-xylitol and β-d-glucosyl-(1,4)-xyllose noticeably stimulated growth yields of L. acidophilus NCFM, and additionally, β-d-glucosyl-(1,4)-xyllose stimulated B. longum Bi-05. α-Glucosyl-(1,4)-glucosamine and α-glucosyl-(1,4)-N-acetyl-glucosamine enhanced the growth rate of B. animalis subsp. lactis and B. longum Bi-05, whereas L. acidophilus NCFM and Bac. vulgatus did not grow on these OS. α-Galactosyl-(1,6)-α-galactosyl-(1,6)-glucose advanced the growth rate of B. animalis subsp. lactis and L. acidophilus NCFM. Thus several of the structurally well-defined OS supported growth of beneficial gut bacteria. This reflects a broad specificity of their sugar transporters for OS, including specificity for non-naturally occurring OS, hence showing promise for design of novel prebiotics.

General information
State: Published
Organisations: National Food Institute, Division of Food Microbiology, Department of Systems Biology, Enzyme and Protein Chemistry, Department of Chemical and Biochemical Engineering, Department of Chemistry, Organic Chemistry, Center for BioProcess Engineering, DuPont Nutrition and Health, Carlsberg Laboratory
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Scopus rating (2015): SJR 1.021 SNIP 1.02 CiteScore 3.15
Web of Science (2015): Indexed yes
Scopus rating (2014): SJR 1.024 SNIP 1.092 CiteScore 3.04
Scopus rating (2013): SJR 1.129 SNIP 1.063 CiteScore 3.29
ISI indexed (2013): ISI indexed yes
Scopus rating (2012): SJR 0.984 SNIP 1.078 CiteScore 2.79
ISI indexed (2012): ISI indexed no
Scopus rating (2011): SJR 0.347 SNIP 0.379 CiteScore 1.14
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Ion Transfer Voltammetry Associated with Two Polarizable Interfaces Within Water and Moderately Hydrophobic Ionic Liquid Systems
An electrochemical system composed of two polarizable interfaces (the metallic electrode|water and water|ionic liquid interfaces), namely two-polarized-interface (TPI) technique, has been proposed to explore the ion transfer processes between water and moderately hydrophobic ionic liquids (W|mIL), typically 1-octyl-3-methylimidazolium bis(trifluoromethylsulfonylimide) (C8mimC1C1N) and 1-hexyl-3-methylimidazolium bis(trifluoromethylsulfonylimide) (C6mimC1C1N). Within the classic four-electrode system, it is not likely that the ion transfer information at the W|mIL interface can be obtained due to an extremely narrow polarized potential window (ppw) caused by these moderately hydrophobic components. In this article, we show that TPI technique has virtually eliminated the ppw limitation based on controlling the step of concentration polarization at the electrode|water interface. With the aid of this technique, the formal ion transfer potential differences between C1C1N– and Cnmim+ (n=6, 8) were accurately determined for 356 mV and 420 mV at a corresponding interface (W|C6mimC1C1N and W|C8mimC1C1N). Besides, this technique is used to monitor
electrochemical polarization at the two W|mIL systems, which exhibits an adaptable polarizability (i.e., a conversion from a nonpolarized interface to a polarized interface). Some of the typical anion transfers at the W/C8mimC1C1N interface have also been investigated, as they are particularly important for ion extraction. The experimental results indicate that this facile TPI technique offers a general avenue to explore ion transfer in multifarious biphasic systems.

**General information**

State: Published  
Organisations: Department of Chemistry, NanoChemistry, Chinese Academy of Sciences  
Authors: Gan, S. (Ekstern), Zhou, M. (Ekstern), Zhang, J. (Intern), Zhong, L. (Ekstern), Ulstrup, J. (Intern), Niu, L. (Ekstern)  
Pages: 857-866  
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Main Research Area: Technical/natural sciences

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BFI (2018): BFI-level 1  
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BFI (2016): BFI-level 1  
Scopus rating (2016): SJR 0.666 SNIP 0.709 CiteScore 2.57  
BFI (2015): BFI-level 1  
Scopus rating (2015): SJR 0.675 SNIP 0.738 CiteScore 2.35  
Web of Science (2015): Indexed yes  
BFI (2014): BFI-level 1  
Scopus rating (2014): SJR 0.674 SNIP 0.773 CiteScore 2.26  
Web of Science (2014): Indexed yes  
BFI (2013): BFI-level 1  
Scopus rating (2013): SJR 0.862 SNIP 0.899 CiteScore 2.74  
ISI indexed (2013): ISI indexed yes  
Web of Science (2013): Indexed yes  
BFI (2012): BFI-level 1  
Scopus rating (2012): SJR 1.114 SNIP 0.865 CiteScore 2.86  
ISI indexed (2012): ISI indexed yes  
BFI (2011): BFI-level 1  
Scopus rating (2011): SJR 1.017 SNIP 0.881 CiteScore 2.86  
ISI indexed (2011): ISI indexed yes  
Web of Science (2011): Indexed yes  
BFI (2010): BFI-level 1  
Scopus rating (2010): SJR 1.084 SNIP 0.852  
BFI (2009): BFI-level 1  
Scopus rating (2009): SJR 1.028 SNIP 0.905  
BFI (2008): BFI-level 1  
Scopus rating (2008): SJR 1.321 SNIP 0.915  
Web of Science (2008): Indexed yes  
Scopus rating (2007): SJR 1.211 SNIP 0.946  
Web of Science (2007): Indexed yes  
Scopus rating (2006): SJR 1.21 SNIP 0.946  
Scopus rating (2005): SJR 1.036 SNIP 0.917  
Scopus rating (2004): SJR 0.986 SNIP 0.9  
Scopus rating (2003): SJR 0.795 SNIP 0.905  
Scopus rating (2002): SJR 1.022 SNIP 0.898
The internal reference oxygen sensor (IROS) based on a binary mixture of metal and its stoichiometric oxide is subject to leaks that result in consumption of the binary mixture. An IROS loses the functionality when the binary mixture is exhausted. Among the possible leak sources the electronic leak of electrolyte is usually unavoidable. Thus, evaluation of the electronic conduction of electrolyte is useful for lifetime estimation. In this study the electronic conduction of 8mol% yttria doped zirconia (8YSZ) that is typically used as the electrolyte for solid oxide cells including the IROSes is evaluated, and the depletion period of an IROS based on the binary mixture of Ni/NIO is discussed. The theoretical prediction of the depletion period is verified by experimental results over more than 6600h. Figures that may be used to predict the depletion period are provided for practical cell design. The electronic conduction of electrolyte can be minimized to make the depletion period of an IROS satisfy the target application up to duration of years.
Ligand binding and activation mechanism of the glucagon-like peptide-1 receptor

In recent years, G-protein coupled receptors (GPCRs) have become important drug targets, which makes elucidation of their molecular structure and functional domains increasingly important for designing new and better therapeutic agents. The Glucagon-Like Peptide-1 receptor (GLP-1R) is a GPCR. Its endogenous agonist, Glucagon-Like Peptide-1 (GLP-1), has a number of physiological effects that contribute to reducing blood sugar and body weight. Therefore, GLP-1R has become a promising target for the treatment of type 2 diabetes (T2D). The overall purpose of the Ph.D. project has been to investigate how GLP-1R interacts with receptor agonists. The thesis includes four studies, which investigate different aspects of these interactions. The first study elucidates GLP-1 binding to the extracellular domain of GLP-1R (ECD) (Study I), whereas the second study identifies receptor domains important for small molecule-mediated activation of GLP-1R (Study II). A fully functional, cysteine-deprived and C-terminally truncated GLP-1R is developed and characterised in Study III. In Study IV, a cAMP biosensor is used to investigate the cAMP kinetics of GLP-1R upon stimulation with different receptor agonists. Collectively, the work has contributed to a more detailed understanding of GLP-1R pharmacology in a number of ways. A crystal structure elucidated the molecular details of GLP-1 binding to the ECD of GLP-1R and supported the existence of different binding modes of GLP-1 and exendin-4. In addition, the work established that seven cysteine residues in GLP-1R and more than half of the C-terminal tail are not required for GLP-1 binding or function. Last but not least, site-directed mutagenesis identified receptor domains and specific residues involved in small molecule-mediated activation of GLP-1R.

General information

State: Published
Organisations: Department of Chemistry, Physical and Biophysical Chemistry, Novo Nordisk A/S
The complex phase equilibrium between reservoir fluids and associating compounds like water and glycols has become more and more important as the increasing global energy demand pushes the oil industry to use advanced methods to increase oil recovery, such as increasing the use of various chemicals to ensure a constant and safe production. The CPA equation of state has been successfully applied in the past to well defined systems and gas condensates, containing associating compounds. It has also been extended to reservoir fluids in presence of water and polar chemicals using modified correlations for critical temperature, pressure and acentric factor. This work presents new phase equilibrium data for binary MEG/reservoir fluid and ternary MEG/water/reservoir fluid systems, where two reservoir fluids from Statoil operated fields are used. The solubility data are reported over a range of temperatures and compositions at atmospheric pressure. The CPA equation of state has been applied to systems containing reservoir fluids, MEG and water. With a minimum number of adjustable parameters from binary pairs, the CPA EoS satisfactorily describes the mutual solubility of the binary systems reservoir fluid and MEG. Promising results are also obtained with CPA EoS for ternary mixtures, with some deviations for the solubility of MEG/water in the hydrocarbon phase and for the hydrocarbons in the polar phase.
Mechanistic Investigation of Palladium–Catalyzed Allylic C–H Activation

The mechanism for the palladium–catalyzed allylic C–H activation was investigated using a combination of experimental and theoretical methods. A Hammett study revealed a buildup of a partial negative charge in the rate-determining step, while determination of the kinetic isotope effect (KIE) indicated that the C–H bond is broken in the turnover-limiting transition state. These experimental findings were further substantiated by carrying out a detailed density functional theory (DFT) based investigation of the entire catalytic cycle. The DFT modeling supports a mechanism where a coordinated acetate acts as a base in an intramolecular fashion during the C–H activation step. The re-oxidation of palladium was found to reach a similar energy level as that of the C–H activation. Calculations of turnover frequencies (TOF) for the entire catalytic cycle for the C–H alkylation were used to acquire a better understanding of the experimental KIE value. The good correspondence between the experimental KIE and the computed KIE values allows a discrimination between the acetate acting in an intramolecular fashion (C–H alkylation) and an intermolecular fashion (C–H acetoxylation and C–H amination).

General information
State: Published
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.
Method for enhancing the thermal stability of ionic compounds
This invention relates to a method for enhancing the thermal stability of ionic compounds including ionic liquids, by immobilization on porous solid support materials having a pore diameter of between about 20-200 AA, wherein the solid support does not have a pore size of 90 AA.

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Authors: Riisager, A. (Intern), Fehrmann, R. (Intern), Robin, R. (Ekstern), Gabriela, G. (Ekstern)
Publication date: 2013
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Patent number: WO2013030299
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Original language: English
Main Research Area: Technical/natural sciences
Publication: Research › Patent – Annual report year: 2011

Method for filling a reactor with a catalyst
The invention relates to a method for filling a reactor with a catalyst for the carbonylation of carbonylated compounds in the gas phase. According to said method, a SILP catalyst is covered with a filling agent which is liquid under normal conditions and is volatile under carbonylation reaction conditions, and a thus-treated catalyst is introduced into the reactor and the reactor is sealed.

General information
State: Published
Organisations: Department of Chemistry, Centre for Catalysis and Sustainable Chemistry
Authors: Zipp, A. (Ekstern), Ruedinger, A. (Ekstern), Fehrmann, R. (Intern), Hanning, C. W. (Ekstern), Riisager, A. (Intern)
Publication date: 2013
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Date: 21/02/2012
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Micro-drilling of polymer tubular ultramicroelectrode arrays for electrochemical sensors
We present a reproducible fast prototyping procedure based on micro-drilling to produce homogeneous tubular ultramicroelectrode arrays made from poly(3,4-ethylenedioxythiophene) (PEDOT), a conductive polymer. Arrays of Ø 100 μm tubular electrodes each having a height of 0.37 ± 0.06 μm were reproducibly fabricated. The electrode dimensions were analyzed by SEM after deposition of silver dendrites to visualize the electroactive electrode area. The electrochemical applicability of the electrodes was demonstrated by voltammetric and amperometric detection of ferricyanide. Recorded signals were in agreement with results from finite element modelling of the system. The tubular PEDOT ultramicroelectrode arrays were modified by prussian blue to enable the detection of hydrogen peroxide. A linear sensor response was demonstrated for hydrogen peroxide concentrations from 0.1 mM to 1 mM.
Minor iridoids from Scutellaria albida ssp albida. Inhibitory potencies on lipoxygenase, linoleic acid lipid peroxidation and antioxidant activity of iridoids from Scutellaria sp

A new iridoid glycoside, 6’-O-E-caffeoyl-mussaenosidic acid, in addition to one known aglycon, four known triterpenes and one known flavonoid, were isolated from the aerial parts of Scutellaria albida subsp. albida. Furthermore, 12 iridoids with similar structures isolated from Scutellaria sp., were examined for their inhibitory potency on lipoxygenase and lipid peroxidation, as well as their antioxidant activity, in comparison to known antioxidants e. g. caffeic acid, nordihydroguaretic acid (NDGA) and trolox. AAPH, DPPH and soybean lipoxygenase (LOX) assays were used for the tests. This investigation led to interesting observations considering the Structure-Activity Relationship. According to our results, the presence of a p-coumaroyl group optimized and even dramatically changed the biological responses of the investigated iridoids.
Modeling degradation in SOEC impedance spectra

Solid oxide cell (SOC) performance is limited by various processes. One way to investigate these processes is by electrochemical impedance spectroscopy. In order to quantify and characterize the processes, an equivalent circuit can be used to model the SOC impedance spectra (IS). Unfortunately, the optimal equivalent circuit is often unknown and to complicate matters further, several processes contribute to the SOC impedance - making detailed process characterization difficult. In this work we analyze and model a series of IS measured during steam electrolysis operation of an SOC. During testing, degradation is only observed in the Ni/YSZ electrode and not in the electrolyte or the LSM/YSZ electrode. A batch fit of the differences between the IS shows that a modified Gerischer element provides a better fit to the Ni/YSZ electrode impedance than the frequently used RQ element - albeit neither equivalent circuit provides a perfect fit. However, modeling with the Gerischer element indicates that the Ni/YSZ electrode performance decrease, relates to an electrochemical reaction resistance increase at the electrode triple phase boundaries. © 2013 The Electrochemical Society.

General information
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Organisations: Department of Energy Conversion and Storage, Applied Electrochemistry, Physical and Biophysical Chemistry, Department of Chemistry, Fundamental Electrochemistry
Authors: Jensen, S. H. (Intern), Hauch, A. (Intern), Knibbe, R. (Intern), Jacobsen, T. (Intern), Mogensen, M. B. (Intern)
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Web of Science (2016): Indexed yes
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Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.151 SNIP 1.299 CiteScore 2.92
Monitoring protein precipitates by in-house X-ray powder diffraction

Powder diffraction from protein powders using in-house diffractometers is an effective tool for identification and monitoring of protein crystal forms and artifacts. As an alternative to conventional powder diffractometers a single crystal diffractometer equipped with an X-ray micro-source can be used to collect powder patterns from 1 l samples. Using a small-angle X-ray scattering (SAXS) camera it is possible to collect data within minutes. A streamlined program has been developed for the calculation of powder patterns from pdb-coordinates, and includes correction for bulk-solvent. A number of such calculated powder patterns from insulin and lysozyme have been included in the powder diffraction database and successfully used for search-match identification. However, the fit could be much improved if peak asymmetry and multiple bulk-solvent corrections were included. When including a large number of protein data sets in the database some problems can be foreseen due to the large number of overlapping peaks in the low-angle region, and small differences in unit cell parameters between pdb-data and powder data. It is suggested that protein entries are supplied with more searchable keywords as protein name, protein type, molecular weight, source organism etc. in order to limit possible hits.

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Nanoscale Confinement and Fluorescence Effects of Bacterial Light Harvesting Complex LH2 in Mesoporous Silicas

Many key chemical and biochemical reactions, particularly in living cells, take place in confined space at the mesoscopic scale. Towards understanding of physicochemical nature of biomacromolecules confined in nanoscale space, in this work we have elucidated fluorescent effects of a light harvesting complex LH2 in nanoscale chemical environments. Mesoporous silicas (SBA-15 family) with different shapes and pore sizes were synthesized and used to create nanoscale biomimetic environments for molecular confinement of LH2. A combination of UV-vis absorption, wide-field fluorescence microscopy and in-situ ellipsometry supports that the LH2 complexes are located inside the silica nanopores. Systematic fluorescence effects were observed and depend on degree of space confinement. In particular, the temperature dependence of the steady-state fluorescence spectra was analyzed in detail using condensed matter bandshape theories. Systematic electronic-vibrational coupling differences in the LH2 transitions between the free and confined states are found, mostly likely responsible for the fluorescence effects experimentally observed.

General information
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Organisations: NanoChemistry, Department of Chemistry, Lund University
Authors: Ikemoto, H. (Intern), Tubasum, S. (Ekstern), Pullerits, T. (Ekstern), Ulstrup, J. (Intern), Chi, Q. (Intern)
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Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.027 SNIP 1.448 CiteScore 5.08
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 2.134 SNIP 1.439 CiteScore 5.14
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 2.514 SNIP 1.46 CiteScore 4.98
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.32 SNIP 1.457 CiteScore 4.92
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 2.438 SNIP 1.356
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Nicotinamide phosphoribosyltransferase inhibitors, design, preparation and SAR.

Existing pharmacological inhibitors for nicotinamide phosphoribosyltransferase (NAMPT) are promising therapeutics for treating cancer. Using medicinal and computational chemistry methods, the structure-activity relationship for novel classes of NAMPT inhibitors is described and compounds optimized. Compounds are designed inspired by the NAMPT inhibitor APO866 and cyanoguanidine inhibitor scaffolds. In comparison with recently published derivatives the new analogues exhibit an equally potent anti-proliferative activity in vitro and comparable activity in vivo. The best performing compounds from these series showed sub-nanomolar anti-proliferative activity towards a series of cancer cell-lines (compound 15: IC50 0.025 nM and 0.33 nM, in A2780 (ovarian carcinoma) and MCF-7 (breast), respectively), and potent anti-tumour in vivo activity in well tolerated doses in a xenograft model. In an A2780 xenograft mouse model with large tumours (500 mm3) compound 15 reduced the tumour volume to one fifth of the starting volume at a dose of 3 mg/kg administered i.p., bid, day 1-9. Thus, compounds found in this study compared favourably with compounds already in the clinic and warrant further investigation as promising lead molecules for the inhibition of NAMPT.

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Nonlinearity in Intensity versus Concentration Dependence for the Deep UV Resonance Raman Spectra of Toluene and Heptane

The relation between Raman scattering, resonance Raman scattering and absorption is reviewed to see to what extent quantitative analysis can be applied in Resonance Raman spectroscopy. In addition to this it is demonstrated experimentally that normal Raman spectra can be dramatically inhibited by absorption and Resonance Raman effects. Raman spectra of toluene and heptane mixtures - with progressively increasing concentrations of heptane - were measured by use of 229 nm excitation. The results show that the characteristic band intensities are not directly proportional to the relative concentrations of the compounds and deviate due to absorption resonance effects. An approximated mathematical model is developed to demonstrate that the intensities of the normal Raman scattering bands are suppressed. An inhibition coefficient $K_i$ is introduced to describe the situation and determine the penetration depth. Most remarkably it is shown that the intensity of the Resonance Raman Scattering bands can be constant even when the concentration ratios differ substantially in the sampled mixtures.
A technique has been developed for the calculation of torsional spring constants for AFM cantilevers based on the combination of the normal spring constant and plate/beam theory. It is easy to apply and allow the determination of torsional constants for stiff cantilevers where the thermal power spectrum is difficult to obtain due to the high resonance frequency and low signal/noise ratio. The applicability is shown to be general and this simple approach can thus be used to obtain torsional constants for any beam shaped cantilever. © 2013 AIP Publishing LLC.
BFI (2017): BFI-level 1
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 1.2 SJR 0.585 SNIP 0.855
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 0.562 SNIP 0.824 CiteScore 1.11
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 0.922 SNIP 1.211 CiteScore 1.45
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 0.898 SNIP 1.117 CiteScore 1.28
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.012 SNIP 1.267 CiteScore 1.45
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.861 SNIP 1.105 CiteScore 1.43
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.214 SNIP 1.415
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.001 SNIP 1.065
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.293 SNIP 1.355
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 0.927 SNIP 1.028
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 1.155 SNIP 1.279
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.876 SNIP 1.058
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.113 SNIP 1.4
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 0.957 SNIP 1.29
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 0.992 SNIP 0.974
Scopus rating (2001): SJR 1.1 SNIP 1.334
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 0.876 SNIP 1.012
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Numerical analysis of a one-dimensional multicomponent model of the in-situ combustion process

An advanced numerical model for the in-situ combustion process is developed and studied in detail. The model is based on further extension and modification of the virtual kinetic cell (VKC) and virtual combustion tube (VCT) developed by Kristensen et al. (2007) and Kristensen (2008). Moreover, the model is based on SARA representation of a petroleum mixture (saturates–aromatics–resins–asphaltenes), which may react differently with oxygen and produce other components (for example, light oils and coke). In total, the model contains 14 components, which may undergo 15 chemical reactions. The set of reactions in the original model of M.R. Kristensen has been modified in order to account for secondary combustion of the light oil fraction. The results of the model implementation are applied to the four heavy oil systems and qualitatively compared to the results of previous experimental studies. A new parameter, the critical ignition saturation, is introduced, in order to describe the easiness of oil ignition. Its dependence on the different parameters of the oil mixture and injection gas is studied. The conclusions on the processes governing the ignition of oil in the presence of water are made. A parameter which affects most the possibility of ignition is the activation energy of the light fraction of the oil.

General information
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Organisations: Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Ressources Engineering, Department of Chemistry
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Scopus rating (2014): SJR 0.692 SNIP 1.751 CiteScore 1.95
Web of Science (2014): Indexed yes
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Scopus rating (2013): SJR 0.822 SNIP 1.901 CiteScore 1.73
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 0.774 SNIP 1.666 CiteScore 1.42
ISI indexed (2012): ISI indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 0.648 SNIP 1.41 CiteScore 1.29
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 0.746 SNIP 1.724
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
O2 Binding to Heme is Strongly Facilitated by Near-Degeneracy of Electronic States

This paper reports the computed O2 binding to heme, which for the first time explains experimental enthalpies for this process of central importance to bioinorganic chemistry. All four spin states along the relaxed FeO2-binding curves were optimized using the full heme system with dispersion, thermodynamic, and scalar-relativistic corrections, applying several density functionals. When including all these physical terms, the experimental enthalpy of O2 binding (−59 kJ mol−1) is closely reproduced by TPSSh-D3 (−66 kJ mol−1). Dispersion changes the potential energy surfaces and leads to the correct electronic singlet and heptet states for bound and dissociated O2. The experimental activation enthalpy of dissociation (∼82 kJ mol−1) was also accurately computed (∼75 kJ mol−1) with an actual barrier height of ∼60 kJ mol−1 plus a vibrational component of ∼10 and ∼5 kJ mol−1 due to the spin-forbidden nature of the process, explaining the experimentally observed difference of ∼20 kJ mol−1 in enthalpies of binding and activation. Most importantly, the work shows how the nearly degenerate singlet and triplet states increase crossover probability up to ∼0.5 and accelerate binding by ∼100 times, explaining why the spin-forbidden binding of O2 to heme, so fundamental to higher life forms, is fast and reversible.

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Organisations: Department of Chemistry, Physical and Biophysical Chemistry
Authors: Kepp, K. P. (Intern)
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Online measurement of mass density and viscosity of pL fluid samples with suspended microchannel resonator

Physical characterization of viscous samples is crucial in chemical, pharma and petroleum industry. For example, in the refining industry of petroleum, water percentage is verified by measuring the density of a sample. In this article we present a suspended microchannel resonator (SMR) which uses 5 pL of a fluid sample and measures its density with a resolution of 0.01 kg/m^3 and a sensitivity of 16 Hz/kg/m^3. The resonator can also simultaneously measure viscosity of the solutions with an accuracy of 0.025 mPa s. The SMR is part of a system which contains packaging and tubing to deliver samples to the resonator. The system can easily handle multiple viscous fluids to measure their densities and viscosities. The SMR is transparent, facilitating visual inspection of the microchannel content. © 2013 Elsevier B.V.
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Organisations: Department of Micro- and Nanotechnology, Nanoprobes, Department of Chemistry, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, Center for Energy Resources Engineering
Authors: Khan, F. (Intern), Schmid, S. (Intern), Larsen, P. E. (Intern), Davis, Z. J. (Intern), Yan, W. (Intern), Stenby, E. H. (Intern), Boisen, A. (Intern)
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Scopus rating (2016): CiteScore 5.07 SJR 1.333 SNIP 1.463
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.25 SNIP 1.509 CiteScore 4.84
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.229 SNIP 1.679 CiteScore 4.37
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
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ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.405 SNIP 1.679 CiteScore 3.92
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.474 SNIP 1.744 CiteScore 4.08
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.409 SNIP 1.437
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.297 SNIP 1.509
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.436 SNIP 1.576
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 1.434 SNIP 1.592
Scopus rating (2006): SJR 1.336 SNIP 1.526
Scopus rating (2005): SJR 1.267 SNIP 1.849
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 1.336 SNIP 1.504
Web of Science (2004): Indexed yes
On the Hopping Efficiency of Nanoparticles in the Electron Transfer across Self-Assembled Monolayers

Redox reactions of solvated molecular species at gold-electrode surfaces modified by electrochemically inactive self-assembled molecular monolayers (SAMs) are found to be activated by introducing Au nanoparticles (NPs) covalently bound to the SAM to form a reactive Au–alkanedithiol–NP–molecule hybrid entity. The NP appears to relay long-range electron transfer (ET) so that the rate of the redox reaction may be as efficient as directly on a bare Au electrode, even though the ET distance is increased by several nanometers. In this study, we have employed a fast redox reaction of surface-confined 6-(ferrocenyl) hexanethiol molecules and NPs of Au, Pt and Pd to address the dependence of the rate of ET through the hybrid on the particular NP metal. Cyclic voltammograms show an increasing difference in the peak-to-peak separation for NPs in the order Au.

General information
State: Published
Organisations: Department of Chemistry, NanoChemistry, Xiamen University
Authors: Liu, F. (Ekstern), Khan, K. (Ekstern), Liang, J. (Ekstern), Yan, J. (Ekstern), Wu, D. (Ekstern), Mao, B. (Ekstern), Jensen, P. S. (Intern), Zhang, J. (Intern), Ulstrup, J. (Intern)
Pages: 952-957
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Main Research Area: Technical/natural sciences
Optimizing the Structure of Tetracyanoplatinate (II): A Comparison of Relativistic Density Functional Theory Methods

The geometry of tetracyanoplatinate(II) (TCP) has been optimized with density functional theory (DFT) calculations in order to compare different computational strategies. Two approximate scalar relativistic methods, i.e. the scalar zeroth-order regular approximation (ZORA) and non-relativistic calculations with relativistic effective core potentials (ECPs), were benchmarked against the four-component fully relativistic approach using the Dirac-Coulomb Hamiltonian and all-electron non-relativistic calculations. We find that the 5% contraction of the platinum-carbon bond due to relativistic effects is almost quantitatively reproduced in the ZORA and ECP calculations. In addition, the effect of the exchange-correlation functional and one-electron basis set was studied by employing the two generalized gradient approximation (GGA) functionals, BLYP and PBE, as well as their hybrid version B3LYP and PBE0 in combination with both correlation consistent and Ahlrichs type basis sets. The platinum-carbon bond length (relativistic or non-relativistic) is approximately 1% shorter on using the PBE exchange-correlation functional compared to the BLYP functional but including exact exchange has no significant effect. For the C-N bond these trends are reversed and an order of magnitude smaller. With respect to the basis set dependence we observed that a triple zeta basis set with polarization functions gives in general sufficiently converged results, but while for the Pt-C bond it is advantageous to include extra diffuse functions, this did not turn out to be important for the C-N bond.

General information
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Organisations: Department of Chemistry, Center for Atomic-scale Materials Design, Physical and Biophysical Chemistry, University of Copenhagen
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**Organic synthesis - applications in enzymatic studies, catalysis and surface modification**

In a desire to explore various areas of synthetic organic chemistry, different projects have been carried out, and each of the four following chapters will describe the work carried out on each of them. The first three chapters are related in some extent and treat the synthesis and biochemical applications of (phospho)lipids, while the last chapter differs and deals with the synthesis and initial structural studies of a C₃ symmetric phosphine oxide.

In the first chapter, a series of phospholipids have been synthesised in order to perform a short structure-activity relationship study of an enzyme, secretory phospholipase A₂ (sPLA₂) capable of hydrolysing phospholipids in the sn-2 position specifically. This enzyme is over-expressed in several types of cancer and is under evaluation as a potential trigger for drug release from a new generation of liposomal drug delivery systems. However, little is known about the steric and electronic requirements in the vicinity of the sn-2 position for an effective hydrolysis catalysed by the enzyme. Based on previous observations and on MD experiments, we developed a theory to predict and/or explain the activity of the enzyme on engineered phospholipids. According to our theory, two aspects of the enzyme-substrate interactions are primordial for an effective hydrolysis to occur: the formation of a constructive Michaelis-Menten complex, and access of water to the hydrolysis site. In order to verify this theory, the synthesised phospholipids were formulated as liposomes and the enzymatic activity was studied. Hydrolysis (or absence of hydrolysis) was monitored by MALDI-TOF-MS. The results observed in these experiments are compared to MD predictions and confirm them.

The second chapter deals with surface functionalization of liposomes. The copper mediated [3+2] azide-alkyne cycloaddition has been successfully applied for this purpose by different groups, but no general optimization has been developed for the reaction on functionalised liposomes. Since the reaction generally takes place between one functionality on the surface of the liposomes membrane and a functionality covalently linked to a coupling partner (such as small molecule, peptide, etc.), we investigated the efficiency of the reaction depending on the position of the functional groups (whether on the liposome or on the coupling partner). Our results indicate that the reaction is most efficient when the liposome carries the alkyne functionality rather than the azide. We also investigated and developed a novel selective method for functionalizing liposomes, which has not yet been reported in the literature, based on the reaction between propargyl-amine decorated liposomes and isothiocyanate derived coupling partners that results in a coupling via formation of an iminothiazolidine.

In the third chapter, the synthesis of sn-2 glyceryl 10,16-dihydroxyhexadecanoate is reported, in the context of the identification of the process of formation of the cutin polymer, one of the primary protective components of the epidermis of land plants. The enzyme responsible for the polymerization (CD₁), as well as its substrate, has been identified, and the role of the enzyme has been demonstrated by its activity on the synthetic dihydroxyacylglycerol.

Finally, the last chapter differs greatly from the first three by its focus: a C₃ symmetric phosphine oxide has been synthesised, which we intend to test, after reduction to the phosphine, as a ligand in organometallic catalysed reactions. The ultimate goal is to obtain enantioselectivity, introduced by the organization of aryl substituents around phosphorous in our ligand.

**General information**

State: Published  
Organisations: Department of Chemistry, Organic Chemistry  
Authors: Viart, H. M. (Intern), Clausen, M. H. (Intern)
Oxidative degradation of acid doped polybenzimidazole membranes and fuel cell durability in the presence of ferrous ions

Phosphoric acid doped polybenzimidazole membranes have been explored as proton exchange membranes for high temperature polymer electrolyte membrane fuel cells. Long-term durability of the membrane is of critical concern and has been evaluated by accelerated degradation tests under Fenton conditions. In this study effects of phosphoric acid and ferrous ions were investigated by measurements of the weight loss, intrinsic viscosity and size exclusion chromatography (SEC) of the polymer membranes. Ferrous ions resulted in, as expected, catalytic formation of peroxide radicals and hence the accelerated polymer degradation in terms of weight loss and molecular weight decrease. The presence of phosphoric acid as an inevitable dopant of the membranes, on the other hand, significantly impeded the membrane degradation by means of metal ion complexing, decreased pH, and acid–base interactions with the amino groups of the polymer. Fuel cell durability tests with contaminations of ferrous ions did show considerable performance degradation, however, primarily due to the catalyst deterioration rather than the membrane degradation.
Photolabile linker for the synthesis of hydroxamic acids

The present invention relates to a photolabile hydroxamate linker based on the o-nitroveratryl group and its application for multistep solid-phase synthesis and controlled photolytic release of hydroxamic acids. The invention provides a method for producing a solid support comprising a hydroxylamine-functionalized photolabile linker, and the so produced hydroxylamine-functionalized photolabile solid support. The invention further provides a method for synthesizing a one-bead-one compound library of hydroxamic acid derivatives on a photolabile linker, as well as a method for screening a library of hydroxamic acid derivatives.

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Authors: Nielsen, T. E. (Intern), Qvortrup, K. (Intern)
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Pooled Calibrations and Retainment of Outliers Improved Chemical Analysis

Analytical chemistry has a large responsibility in society, and credibility and reliability are important concepts associated with chemical analysis. Metrology and Quality Assurance (QA) are key areas of interest in contemporary research. Quality in measurements is illustrated by a series of experiments with several analytical technologies comprising ICP-MS, GC-MS and AAS. The scientific methodology relies on the concept of reproducibility that depends on the type of analyte and type of apparatus. By applying the principle of pooled calibrations it is shown that the performance of the apparatus in terms of levels of uncertainty can be tested in a single laboratory. The uncertainties are compared to predictions of the Horwitz formula. It is suggested that this method is universally applicable not only to the actual technologies but also to other technologies in other fields of science. The results indicate that the procedures outlined in the Eurachem/CITAC
Guide are of tremendous value to analytical sciences because they direct researcher’s attention towards the concept of consensus values rather than towards true values. Introduction of certified reference materials (CRM’s) in metrology has provided much new information on working habits in professional laboratories and CRM’s may be applied to establish the true level of uncertainty for a given type of analytical method. Finally, it is proposed to devise a new procedure of method validation that facilitates QA in general, thus saving many resources at laboratories.

General information
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Organisations: Department of Chemistry, Analytical Chemistry, Aarhus University
Authors: Andersen, J. (Intern), Sattar Hassan Alfaloje, H. (Ekstern)
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Scopus rating (2013): SJR 0.197 SNIP 0.32 CiteScore 0.53
ISI indexed (2013): ISI indexed yes
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Scopus rating (2012): SJR 0.204 SNIP 0.285 CiteScore 0.39
ISI indexed (2012): ISI indexed yes
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ISI indexed (2011): ISI indexed yes
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Scopus rating (2008): SJR 0.189 SNIP 0.345
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Scopus rating (2002): SJR 0.199 SNIP 0.371
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Scopus rating (1999): SJR 0.193 SNIP 0.407
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Positively selected sites in cetacean myoglobins contribute to protein stability.

Since divergence ∼50 Ma ago from their terrestrial ancestors, cetaceans underwent a series of adaptations such as a ∼10-20 fold increase in myoglobin (Mb) concentration in skeletal muscle, critical for increasing oxygen storage capacity and prolonging dive time. Whereas the O2-binding affinity of Mbs is not significantly different among mammals (with typical oxygenation constants of ∼0.8-1.2 µM(-1)), folding stabilities of cetacean Mbs are ∼2-4 kcal/mol higher than for terrestrial Mbs. Using ancestral sequence reconstruction, maximum likelihood and Bayesian tests to describe the evolution of cetacean Mbs, and experimentally calibrated computation of stability effects of mutations, we observe accelerated evolution in cetaceans and identify seven positively selected sites in Mb. Overall, these sites contribute to Mb stabilization with a conditional probability of 0.8. We observe a correlation between Mb folding stability and protein abundance, suggesting that a selection pressure for stability acts proportionally to higher expression. We also identify a major divergence event leading to the common ancestor of whales, during which major stabilization occurred. Most of the positively selected sites that occur later act against other destabilizing mutations to maintain stability across the clade, except for the shallow divers, where late stability relaxation occurs, probably due to the shorter aerobic dive limits of these species. The three main positively selected sites 66, 5, and 35 undergo changes that favor hydrophobic folding, structural integrity, and intra-helical hydrogen bonds.
Prediction of the vapor–liquid equilibria and speed of sound in binary systems of 1-alkanols and n-alkanes with the simplified PC-SAFT equation of state

Prediction of speed of sound is a challenging task for any equation of state because it needs the first- and second-order derivatives of the Helmholtz free energy with respect to both temperature and volume. Equally challenging is the simultaneous predictions of phase behavior and speed of sound (or other derivative properties) with satisfactory accuracy over wide temperature, pressure and composition conditions. This work presents the prediction of the vapor–liquid equilibria and speed of sound in binary mixtures of 1-alkanols and n-alkanes using the simplified PC-SAFT equation of state with pure component parameters estimated in different ways. All results are straight predictions, i.e. no binary interaction parameters are used. With the parameters presented in this work, the predicted overall percent average absolute deviations are, respectively, around 6.1% for the saturation pressure for 1533 experimental data points in the temperature range from 273 to 493K, and 1.7% for the speed of sound for 2490 experimental data points at temperature between 293 and 318K and pressure up to 120MPa. The results reveal that it is possible to simultaneously model the vapor–liquid equilibria and speed of sound with a satisfactory accuracy for 1-alkanols and n-alkanes binary systems within the PC-SAFT framework.
PTH (1–34), but not strontium ranelate counteract loss of trabecular thickness and bone strength in disuse osteopenic rats

PTH and strontium ranelate (SrR) have both been shown to reduce bone loss induced by immobilization. PTH is a potent bone anabolic agent, whereas SrR has been suggested to be an antiresorptive as well as a bone anabolic agent. The aim of the study was to investigate whether PTH, SrR, and PTH and SrR in combination could counteract immobilization-induced bone loss in a rat model. Immobilization was induced by injecting 4IU Botox (BTX) into the muscles of the right hind limb. Seventy-two female Wistar rats, 3-months-old, were divided into the following groups: Baseline, Controls, BTX, BTX+PTH, BTX+SrR, and BTX+PTH+SrR (n=12 in each group). PTH was given as injections (SC) at a dosage of 60 μg/kg/d, and SrR as 900 mg/kg/d in the diet. The experiment lasted for 4 weeks. BTX resulted in lower trabecular bone formation rate (−68%) and periosteal bone formation rate (−91%), and a higher fraction of osteoclast-covered surfaces (+53%) compared with controls. This was accompanied by significantly lower trabecular bone volume fraction (−24%), trabecular thickness (−16%), and bone strength (−14% to −32% depending on site). PTH alone counteracted immobilization-induced losses in trabecular bone formation rate (+24% vs. BTX) and periosteal bone formation rate (+14% vs. BTX). In contrast, SrR did not
influence BTX-induced loss of bone formation rate, trabecular bone volume fraction, trabecular thickness, or bone strength. Finally, no additive effect was found when PTH and SrR treatments were combined. In conclusion, PTH counteracted loss in bone architecture and bone strength in immobilized rats, whereas no effect of SrR was found. Moreover, no additional effect was found by combining PTH with SrR.

General information
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Authors: Brüel, A. (Forskerdatabase), Vegger, J. B. (Forskerdatabase), Raffalt, A. C. (Intern), Andersen, J. (Intern), Thomsen, J. S. (Ekstern)
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Scopus rating (2014): SJR 1.794 SNIP 1.656 CiteScore 4.18
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ISI indexed (2013): ISI indexed yes
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BFI (2011): BFI-level 1
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Scopus rating (2010): SJR 1.785 SNIP 1.657
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.759 SNIP 1.593
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.848 SNIP 1.515
Scopus rating (2007): SJR 1.841 SNIP 1.52
Scopus rating (2006): SJR 1.758 SNIP 1.517
Scopus rating (2005): SJR 1.671 SNIP 1.646
Scopus rating (2004): SJR 1.329 SNIP 1.483
Scopus rating (2003): SJR 1.456 SNIP 1.344
Scopus rating (2002): SJR 1.511 SNIP 1.551
Scopus rating (2001): SJR 1.479 SNIP 1.666
Scopus rating (2000): SJR 1.411 SNIP 1.438
Scopus rating (1999): SJR 1.323 SNIP 1.58
Pulling the levers of photophysics

General information
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Organisations: Department of Chemistry, University of Copenhagen
Authors: Kuhlman, T. S. (Intern), Pittelkow, M. (Ekstern), Sølling, T. I. (Intern), Møller, K. B. (Intern)
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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
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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
Pulling the Levers of Photophysics: How Structure Controls the Rate of Energy Dissipation

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Organisations: Physical and Biophysical Chemistry, Department of Chemistry, University of Copenhagen
Authors: Kuhlman, T. S. (Intern), Pittelkow, M. (Forskerdatabase), Sølling, T. I. (Ekstern), Møller, K. B. (Intern)
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Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
ISI indexed (2011): ISI indexed no
BFI (2010): BFI-level 1
### Purification of 5-hydroxymethylfurfural (hmf) by crystallization

This invention relates to an efficient procedure for purifying HMF by crystallization at low temperature from an organic solvent.

### Quantitative studies of antimicrobial peptide-lipid membrane interactions

The increasing occurrence of multi-drug-resistant bacteria poses a serious threat to modern society. Therefore, novel types of anti-infective therapeutics are highly warranted. Antimicrobial peptides are a class of naturally occurring host-defense molecules that potentially might be developed into such novel therapeutics. However, limited understanding of the mechanisms underlying microbicidal activity of antimicrobial peptides has slowed down this development. A central step toward understanding the microbicidal mechanisms of action of antimicrobial peptides is to understand the mechanisms by which antimicrobial peptides interact with phospholipid membranes. Motivated by that fact, the scope of this thesis is to study these antimicrobial peptide-lipid membrane interactions. In particular, we attempt to study these interactions with a quantitative approach. For that purpose, we consider the three archetypal α-helical antimicrobial peptides mastoparan X, melittin, and magainin 2 as model peptides. These three peptides are investigated by three different experimental techniques.

The first of these experimental techniques is analytical HPLC. We use this technique to document an effect that might pose a significant problem for quantitative studies of antimicrobial peptide-lipid membrane interactions; namely that antimicrobial peptides adsorb to surfaces of glass and plastic. Specifically, we demonstrate that under standard experimental conditions, this effect is significant for mastoparan X, melittin and magainin 2. Consequently, we conclude that investigators should always take this adsorptive effect into account when designing and interpreting their experiments on antimicrobial peptides.

The second experimental technique is fluorescence correlation spectroscopy (FCS). We use this technique to document an effect that might pose a significant problem for quantitative studies of antimicrobial peptide-lipid membrane interactions; namely that antimicrobial peptides adsorb to surfaces of glass and plastic. Specifically, we demonstrate that under standard experimental conditions, this effect is significant for mastoparan X, melittin and magainin 2. Consequently, we conclude that investigators should always take this adsorptive effect into account when designing and interpreting their experiments on antimicrobial peptides.

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formed by antimicrobial peptides. We demonstrate the applicability of FCS by using the technique to study partial transient leakage induced by mastoparan X, melittin, and magainin 2. The leakage data demonstrate that magainin 2 forms larger and/or more stable transmembrane pores in POPC/POPG (3:1) lipid bilayers than do mastoparan X and melittin.

The third and final technique is confocal imaging. Specifically, we use this technique to visualize fluorescently-labeled surface-tethered large unilamellar lipid vesicles. We design an experimental protocol that allows us to directly correlate antimicrobial peptide-induced leakage of fluorescent markers from these surface-tethered vesicles to antimicrobial peptide-induced leakage of fluorescent markers from lipid vesicles in solution. Thereby, we have developed a direct and flexible approach for quantitative evaluation of antimicrobial peptide-induced leakage from large unilamellar lipid vesicles on the single-vesicle level, allowing us an unprecedented level of insight into the leakage process. For example, the surface-tethered lipid vesicles can be used to directly visualize how the single-vesicle leakage profiles depend on the marker size. We employ the surface-tethered vesicles to study partial transient leakage induced by mastoparan X, melittin and magainin 2 from POPC/POPG (3:1) large unilamellar lipid vesicles. The results show that on the single-vesicle level, all three peptides induce heterogeneous leakage in the sense that they induce complete emptying of some vesicles and only partly emptying of other vesicles. This heterogeneous leakage profile is observed regardless of the size of the lumen dye.
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Web of Science (2018): Indexed yes
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BFI (2016): BFI-level 1
Scopus rating (2016): CiteScore 3.06 SJR 1.946 SNIP 1.018
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 2.145 SNIP 1.173 CiteScore 3.3
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 2.203 SNIP 1.166 CiteScore 3.33
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 2.229 SNIP 1.165 CiteScore 3.64
ISI indexed (2013): ISI indexed yes
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Scopus rating (2012): SJR 2.343 SNIP 1.154 CiteScore 3.57
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Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 2.322 SNIP 1.204 CiteScore 3.75
ISI indexed (2011): ISI indexed yes
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Scopus rating (2009): SJR 2.953 SNIP 1.361
Web of Science (2009): Indexed yes
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Scopus rating (2008): SJR 3.222 SNIP 1.416
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 3.119 SNIP 1.422
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 2.807 SNIP 1.416
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Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 2.617 SNIP 1.428
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 2.508 SNIP 1.45
Web of Science (2002): Indexed yes
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Web of Science (2001): Indexed yes
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Quantum-dynamical Modeling of the Rydberg to Valence Excited-State Internal Conversion in Cyclobutanone and Cyclopentanone

In this paper we present 4-state, 5-dimensional Vibronic Coupling Hamiltonians for cyclobutanone and cyclopentanone. Wave packet calculations using these Hamiltonians reveal that for cyclobutanone the (n,3s) to (n,π*) internal conversion involves direct motion in nuclear modes coupling the two states leading to fast population transfer. For cyclopentanone, internal vibrational energy redistribution is a bottleneck for activating reactive nuclear modes leading to slower population transfer.

General information
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Authors: Kuhlman, T. S. (Intern), Sauer, S. P. A. (Forskerdatabase), Solling, T. I. (Ekstern), Møller, K. B. (Intern)
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Main Research Area: Technical/natural sciences

Quartz Crystal Microbalance with Dissipation (QCM-D) studies of the viscoelastic response from a continuously growing grafted polyelectrolyte layer

Poly(acrylic acid) was grown from substrates by photopolymerization, and the grafting process was monitored in situ by Quartz Crystal Microbalance with Dissipation (QCM-D) measurements in a 1:1 v/v mixture of water/ethanol. The polymerization process was monitored into the thick film region, where the change in frequency and dissipation with increasing film mass changes sign as predicted by the Voigt viscoelastic model. Our experimental data are compared with predictions of this model, and satisfactory agreement is found for low overtone numbers. The Voigt model was applied to analyze the measured changes in frequency, Δf, and dissipation, ΔD, in order to extract information on layer thickness, shear elasticity, μ, and shear viscosity, η, of the growing film. The increasing rate of changes in Δf and ΔD observed after about 150 s of polymerization was found to correlate with an increasing growth rate of the film thickness. For longer
polymerization times a close to linear increase in thickness with time was observed. The sensitivity, defined as the derivatives of $\Delta f$ and $\Delta D$ with respect to thickness, depends on overtone number and is different for the frequency and dissipation signals - facts that should be considered when investigating small changes in thick films used in e.g. sensor applications. © 2013 Elsevier Inc.

**General information**

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Authors: Dunér, G. (Ekstern), Thormann, E. (Intern), Dedinaite, A. (Ekstern)
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Scopus rating (2016): CiteScore 4.14 SJR 1.144 SNIP 1.267
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): SJR 1.095 SNIP 1.263 CiteScore 3.8
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): SJR 1.166 SNIP 1.406 CiteScore 3.74
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
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ISI indexed (2013): ISI indexed yes
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Scopus rating (2012): SJR 1.298 SNIP 1.469 CiteScore 3.4
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
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ISI indexed (2011): ISI indexed yes
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Scopus rating (2010): SJR 1.279 SNIP 1.46
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BFI (2009): BFI-level 1
Scopus rating (2009): SJR 1.207 SNIP 1.4
Web of Science (2009): Indexed yes
BFI (2008): BFI-level 1
Scopus rating (2008): SJR 1.144 SNIP 1.335
Scopus rating (2007): SJR 1.026 SNIP 1.369
Web of Science (2007): Indexed yes
Scopus rating (2006): SJR 0.992 SNIP 1.366
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 0.984 SNIP 1.365
Real-Time DNP NMR Observations of Acetic Acid Uptake, Intracellular Acidification, and of Consequences for Glycolysis and Alcoholic Fermentation in Yeast

Uptake and upshot in vivo: Straightforward methods that permit the real-time observation of organic acid influx, intracellular acidification, and concomitant effects on cellular-reaction networks are crucial for improved bioprocess monitoring and control (see scheme). Herein, dynamic nuclear polarization (DNP) NMR is used to observe acetate influx, ensuing intracellular acidification and the metabolic consequences on alcoholic fermentation and glycolysis in living cells.

General information
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Authors: Jensen, P. R. (Intern), Karlsson, M. (Intern), Lerche, M. H. (Intern), Meier, S. (Intern)
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Web of Science (2017): Indexed yes
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Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
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Regioselective Glycosylation of Unprotected Phenyl 1-Thioglycopyranosides with Phenylboronic Acid as a Transient Masking Group

A useful protocol is described for the regioselective glycosylation of the secondary alcohols in unprotected glycosyl acceptors. Phenyl 1-thioglycopyranosides derived from D-glucose, D-galactose, D-glucosamine, L-rhamnose, and L-fucose were treated with phenylboronic acid to install a temporary boronic ester, and then submitted to a Koenigs–Knorr glycosylation with perbenzoylated glucopyranosyl or galactopyranosyl bromides. Good yields for coupling to the 3-position in glucosides and galactosides were achieved, but lower yields were obtained with the other acceptors. With phenyl 1-thio-β-D-glucopyranoside, the coupling could also be achieved with a superarmed thiogalactoside donor. The product from a glucose–glucose coupling could be subjected to a second regioselective glycosylation at the 6-position. In the galactose series, a β(1→3)-linked galactotriose could be prepared in good yield by two consecutive glycosylations in one pot, where a free 2-hydroxy group ensures neighboring group participation in the second coupling.
Response to Letter to the Editor regarding the "European Analytical Column No. 41"

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Web of Science (2016): Indexed yes
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Web of Science (2015): Indexed yes
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Scopus rating (2014): SJR 1.126 SNIP 1.222 CiteScore 3.26
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 1
Scopus rating (2013): SJR 1.229 SNIP 1.282 CiteScore 3.55
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Web of Science (2013): Indexed yes
BFI (2012): BFI-level 1
Scopus rating (2012): SJR 1.347 SNIP 1.282 CiteScore 3.51
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 1
Scopus rating (2011): SJR 1.363 SNIP 1.275 CiteScore 3.47
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 1
Scopus rating (2010): SJR 1.354 SNIP 1.236
Revisiting the Brønsted acid catalysed hydrolysis kinetics of polymeric carbohydrates in ionic liquids by in situ ATR-FTIR spectroscopy

A new versatile method to measure rates and determine activation energies for the Brønsted acid catalysed hydrolysis of cellulose and cellobiose (and other polymeric carbohydrates) in ionic liquids is demonstrated by following the C–O stretching band of the glycoside bond with in situ ATR-FTIR. An activation energy in excellent agreement with the literature was determined for cellulose hydrolysis, whereas a distinctly lower activation energy was determined for cellobiose hydrolysis. The methodology also allowed to independently determine activation energies for the formation of 5-hydroxymethylfurfural in the systems.

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Organisations: Centre for Catalysis and Sustainable Chemistry, Department of Chemistry
Authors: Kunov-Kruse, A. J. (Intern), Riisager, A. (Intern), Shunmugavel, S. (Intern), Berg, R. W. (Intern), Kristensen, S. B. (Intern), Fehrmann, R. (Intern)
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Web of Science (2015): Indexed yes
Ruthenium-catalyzed self-coupling of primary and secondary alcohols with the liberation of dihydrogen

The dehydrogenative self-condensation of primary and secondary alcohols has been studied in the presence of RuCl2(lrPr)(p-cymene). The conversion of primary alcohols into esters has been further optimized by using magnesium nitride as an additive, which allows the reaction to take place at a temperature and catalyst loading lower than those described previously. Secondary alcohols were dimerized into racemic ketones by a dehydrogenative Guerbet reaction with potassium hydroxide as the additive. The transformation gave good yields of the ketone dimers with a range of alkan-2-ols, whereas more substituted secondary alcohols were unreactive. The reaction proceeds by dehydrogenation to the ketone, followed by an aldol reaction and hydrogenation of the resulting enone. © 2013 American Chemical Society.

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry
Authors: Makarov, I. (Intern), Madsen, R. (Intern)
Ruthenium-Catalyzed Transformations of Alcohols: Mechanistic Investigations and Methodology Development

The mechanism of the ruthenium-catalyzed dehydrogenative synthesis of amides from alcohols and amines was studied in detail by employing the combination of experimental and theoretical techniques. The Hammett study revealed that a small positive charge is formed at the benzylic position in the transition state of the turnover-determining step. The value of the kinetic isotope effect of 2.29 \pm 0.15 indicated that the C–H bond breakage is not the rate-determining step, but that it is one of several slow steps in the catalytic cycle. Experiments with deuterium-labeled alcohols and amines revealed that ruthenium-dihydride species are involved in the catalytic cycle. These experimental results were used in the dft/m06 computational study and a plausible catalytic cycle was proposed. Both cis-dihydride and transdihydride intermediates were considered, but when the theoretical turnover frequencies were obtained from the calculated energies, it was found that only the trans-dihydride pathway was in agreement with the experimentally determined frequencies. The proposed catalytic cycle was used for an in silico search for more effective carbene ligands. The study showed that the ruthenium complexes with dimethoxyisopropylidene and pyridilidene ligands could be more active than RuCl2(IiPr)(p-cymene) used in the mechanistic investigation. Two analogs of the calculated complexes were synthesized but were not isolated in a pure form. The amidation reaction catalyzed by a mixture containing the N-ethyl pyridilidene-substituted ruthenium complex afforded the amide in 38% yield. It indicated that in silico ligand screening might be used for catalyst optimization if it is combined with a more comprehensive experimental study. An improved protocol was developed for the ruthenium-catalyzed dehydrogenative self-coupling of primary alcohols to give esters. Addition of 16.7 mol% of Mg3N2 to the reaction mixture gave esters from aliphatic alcohols in similar yields but at lower temperature as compared with previously a reported catalytic system. This additive also suppressed the decarbonylation of aromatic alcohols. A previously unknown ruthenium-catalyzed dehydrogenative Guerbet reaction with secondary alcohols to give ketones was discovered. The reaction conditions were optimized and the scope and the limitations were studied. It was found that only acyclic 2-methyl carbinols and simple cyclic alcohols underwent this transformation. It was shown that the reaction proceeded via the oxidation–aldol condensation–reduction pathway and that the active ruthenium species was a dihydride. During the external stay at Haldor Topsee A/S, the transformation of acetaldehyde over zeolite-type heterogeneous catalysts was studied. It was shown that tin-Beta zeolite was only capable of producing crotonaldehyde in low yields. Several other heterogeneous catalysts were tested (Al-Beta, Ti-Beta, Sn-MCM-41, ts-1) but none of them demonstrated substantially higher activity in the studied transformation.
Ruthenium Hydride/Brønsted Acid-Catalyzed Tandem Isomerization/N-Acyliminium Cyclization Sequence for the Synthesis of Tetrahydro-β-carbolines

This paper describes an efficient tandem sequence for the synthesis of 1,2,3,4-tetrahydro-β-carbolines (THBCs) relying on a ruthenium hydride/Brønsted acid-catalyzed isomerization of allylic amides to N-acyliminium ion intermediates which are trapped by a tethered indolenucleophile. The methodology provides not only a convenient "aldehyde-free" alternative to the classical Pictet–Spengler reaction but also attractive possibilities for total synthesis, including rapid generation of molecular complexity and formation of quaternary stereogenic centers. TBHCs can also be accessed by harnessing the Suzuki cross-coupling reaction to the isomerization/N-acyliminium cyclization sequence. Finally, diastereo- and enantioselective versions of the title reaction have been examined using substrate control (with dr >15: 1) and asymmetric catalysis (ee up to 57%), respectively.

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Scopus rating (2016): CiteScore 4.59 SJR 1.976 SNIP 1.03
Web of Science (2016): Indexed yes
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Scopus rating (2014): SJR 2.003 SNIP 1.222 CiteScore 4.69
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Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
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BFI (2011): BFI-level 2
Scopus rating (2011): SJR 2.27 SNIP 1.261 CiteScore 4.43
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 2.112 SNIP 1.173
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Scopus rating (2009): SJR 2.186 SNIP 1.254
Web of Science (2009): Indexed yes
Selective production of aromatics from alkylfurans over solid acid catalysts

Solid acid catalysts were studied at temperatures near 523K for the production of benzene, toluene, and p-xylene by the reaction of ethylene with furan, 2-methylfuran, and 2,5-dimethylfuran, respectively, through the combination of cycloaddition and dehydrative aromatization reactions. Catalysts containing Brønsted acid and Lewis acid sites (i.e., WOx-ZrO2, niobic acid, zeoliteY, silica-alumina) were more active than catalysts containing predominantly Lewis acid sites (γ-Al2O3, TiO2), which indicates the importance of Brønsted acidity in the production of aromatics. Microporosity is not required for this reaction, because amorphous solid acids and homogeneous Brønsted acids demonstrate significant activity for p-xylene production. The production of p-xylene from 2,5-dimethylfuran proceeded at higher rates compared with the production of toluene and benzene from 2-methylfuran and furan, respectively. Both WOx-ZrO2 and niobic acid demonstrate superior activity for aromatics production than does zeoliteY. WOx-ZrO2 demonstrated a turnover frequency for p-xylene production that is 35 times higher than that demonstrated by zeoliteY. In addition, mesoporous materials such as WOx-ZrO2 offer higher resistance to deactivation by carbon deposition than do microporous materials. Results from Raman spectroscopy and the trend of turnover frequency with varying tungsten surface densities for a series of WOx-ZrO2 catalysts are consistent with previous investigations of other acid-catalyzed reactions; this suggests that the high reactivity of WOx-ZrO2 is mainly associated with the presence of subnanometer WOx clusters mixed with zirconium, which reach a maximum surface concentration at intermediate tungsten coverage.

General information

State: Published
Organisations: Department of Chemistry, Department of Physics, University of Wisconsin-Madison, Haldor Topsoe AS
Authors: Wang, D. (Forskerdatabase), Dumesic, J. A. (Ekstern), Osmundsen, C. M. (Intern), Taarning, E. (Ekstern), Osmundsen, C. M. (Intern)
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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.

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Short-term algal testing – a new approach for disclosing silver nanoparticle toxicity

General information
State: Published
Organisations: Department of Environmental Engineering, Department of Chemistry, NanoChemistry, Technical University of Denmark
Authors: Sørensen, S. N. (Intern), Laurelle, S. (Ekstern), Engelbrekt, C. (Intern), Baun, A. (Intern)
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Short-term algal testing – a new approach for disclosing silver nanoparticle toxicity

General information
State: Published
Organisations: Department of Environmental Engineering, Department of Chemistry, NanoChemistry, Technical University of Denmark
Authors: Sørensen, S. N. (Intern), Laurelle, S. (Ekstern), Baun, A. (Intern), Engelbrekt, C. (Intern)
Number of pages: 1
Solid-phase iminium cyclization reactions for the synthesis of natural product-like diketopiperazines

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Organisations: Department of Chemistry, Organic Chemistry
Authors: Petersen, R. (Intern), Le Quement, S. T. (Intern), Nielsen, T. E. (Intern)
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Web of Science (2013): Indexed yes
Scopus rating (2012): SJR 0.1 SNIP 0
Scopus rating (2011): SJR 0.101 SNIP 0
Web of Science (2011): Indexed yes
Scopus rating (2010): SJR 0.101 SNIP 0
Scopus rating (2009): SJR 0.101 SNIP 0
BFI (2008): BFI-level 1
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Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 0.111 SNIP 0.008
Scopus rating (2002): SJR 0.115 SNIP 0.046
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Solving inverse problems through a smooth formulation of multiple-point geostatistics
In oil and gas sector accurate reservoir description play a crucial role in problems associated with recovery of hydrocarbons, risk estimation and predicting reservoir performance. Knowledge on reservoir properties can be inferred from measurements typically made at the surface by solving corresponding inverse problems. However, noise in data, non-linear relationships and sparse observations impede creation of realistic reservoir models. Including complex a priori information on reservoir parameters facilitates the process of obtaining acceptable solutions. Such a priori knowledge may be inferred, for instance, from a conceptual geological model termed a training image. The main motivation for this study was the challenge posed by history matching, an inverse problem aimed at estimating rock properties from production data. We addressed two main difficulties of the history matching problem: existence of multiple, most often geologically unfeasible, solutions and high computational cost of the forward simulation. The developed methodology resulted in a new method for solving inverse problems with training-image based a priori information, when the computational time matters. Specifically, we have proposed a smooth formulation of training-image based priors, which was inspired by the Frequency Matching method developed by our group earlier. The proposed smooth generalization, that integrates data and multiple-point statistics in a probabilistic framework, allows us to find solution by use of gradient-based optimization. As the result, solutions to an inverse problem may be obtained efficiently by deterministic search. We have applied the proposed methodology to the problem of history matching. Both the smooth formulation and the Frequency Matching method find the solution by maximizing its posterior probability. This is achieved by introducing a closed form expression for the a priori probability density. We have defined an expression for the training-image based prior by applying the theory of multinomial distributions. Its combination with the likelihood function results in the closed form expression for defining relative posterior probabilities of the solutions. Finally, we applied the developed smooth formulation to the problem of seismic inversion. The proposed methodology allows us to invert seismic reflection data for rock properties, namely for porosity, by integrating rock physics model into inversion procedure. Errors associated with conversion from depth to time are handled with a novel mapping approach. This thesis reviews the latest developments in the field of geoscience with a focus on the history matching problem. The work contains detailed explanation of our strategies including both theoretical motivation and practical aspects of implementation. Finally, it is complemented by six research papers submitted, reviewed and/or published in the period 2010 - 2013.

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Organisations: National Space Institute, Center for Energy Resources Engineering, Department of Chemical and Biochemical Engineering, CERE – Center for Energy Resources Engineering, Department of Chemistry
Authors: Melnikova, Y. (Intern), Mosegaard, K. (Intern), Shapiro, A. (Intern), Stenby, E. H. (Intern)
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Publication: Research › Ph.D. thesis – Annual report year: 2014

Speeding up compositional reservoir simulation through an efficient implementation of phase equilibrium calculation
Compositional reservoir simulations are widely used to simulate reservoir processes with strong compositional effects, such as gas injection. The equations of state (EoS) based phase equilibrium calculation is a time consuming part in this type of simulations. The phase equilibrium problem can be either decoupled from or coupled with the transport problem. In the former case, flash calculation is required, which consists of stability analysis and subsequent phase split calculation; in the latter case, no explicit phase split calculation is required but efficient stability analysis and optimized coding of the basic thermodynamic subroutines are still crucial to the overall speed. This work tries to provide a comprehensive strategy to increase the speed for compositional simulation. This strategy begins with the coding of the basic thermodynamic properties, including the derivatives of fugacities with respect to molar numbers. Then, in the algorithms for stability analysis and phase split calculation, successive substitution with acceleration and minimization-based second-order methods are combined to gain both robustness and efficiency. For compositional simulations, the results from previous simulation steps provide the possibility to skip stability analysis by the shadow region method in the single phase regions. The approach was implemented in the general purpose research simulator (GPRS) developed by Stanford University. GPRS is a modular, state-of-the-art reservoir simulation and its architecture makes the implementation and evaluation of new ideas and concepts easy. Tests on several 2-D and 3-D gas injection examples indicate that with an efficient implementation of the thermodynamic package and the conventional stability analysis algorithm, the speed can be increased by several folds. Application of the shadow region method to skip stability analysis can further cut the phase equilibrium calculation time. Copyright 2013, Society of Petroleum Engineers.

General information
State: Published
Organisations: Center for Energy Resources Engineering, CERE – Center for Energy Resources Engineering, Department of Chemistry, Department of Chemical and Biochemical Engineering, Eni, University of Bergen
Stability mechanisms of a thermophilic laccase probed by molecular dynamics.

Laccases are highly stable, industrially important enzymes capable of oxidizing a large range of substrates. Causes for their stability are, as for other proteins, poorly understood. In this work, multiple-seed molecular dynamics (MD) was applied to a Trametes versicolor laccase in response to variable ionic strengths, temperatures, and glycosylation status. Near-physiological conditions provided excellent agreement with the crystal structure (average RMSD ~0.92 Å) and residual agreement with experimental B-factors. The persistence of backbone hydrogen bonds was identified as a key descriptor of structural response to environment, whereas solvent-accessibility, radius of gyration, and fluctuations were only locally relevant. Backbone hydrogen bonds decreased systematically with temperature in all simulations (~9 per 50 K), probing structural changes associated with enthalpy-entropy compensation. Approaching T opt (~350 K) from 300 K, this change correlated with a beginning "unzipping" of critical β-sheets. 0 M ionic strength triggered partial denucleation of the C-terminal (known experimentally to be sensitive) at 400 K, suggesting a general salt stabilization effect. In contrast, F(-) (but not Cl(-)) specifically impaired secondary structure by formation of strong hydrogen bonds with backbone NH, providing a mechanism for experimentally observed small anion destabilization, potentially remedied by site-directed mutagenesis at critical intrusion sites. N-glycosylation was found to support structural integrity by increasing persistent backbone hydrogen bonds by ~4 across simulations, mainly via prevention of F(-) intrusion. Hydrogen-bond loss in distinct loop regions and ends of critical β-sheets suggest potential strategies for laboratory optimization of these industrially important enzymes.
Stability Mechanisms of Laccase Isoforms using a Modified FoldX Protocol Applicable to Widely Different Proteins

A recent computational protocol that accurately predicts and rationalizes protein multisite mutant stabilities has been extended to handle widely different isoforms of laccases. We apply the protocol to four isoenzymes of Trametes versicolor laccase (TvL) with variable lengths (498–503 residues) and thermostability (Topt ∼ 45–80 °C) and with 67–77% sequence identity. The extended protocol uses (i) statistical averaging, (ii) a molecular-dynamics-validated “compromise” homology model to minimize bias that causes proteins close in sequence to a structural template to be too stable due to having the benefits of the better sampled template (typically from a crystal structure), (iii) correction for hysteresis that favors the input template to overdestabilize, and (iv) a preparative protocol to provide robust input sequences of equal length. The computed ΔΔG values are in good agreement with the major trends in experimental stabilities; that is, the approach may be applicable for fast estimates of the relative stabilities of proteins with as little as 70% identity, something that is currently extremely challenging. The computed stability changes associated with variations are Gaussian-distributed, in good agreement with experimental distributions of stability effects from mutation. The residues causing the differential stability of the four isoforms are consistent with a range of compiled laccase wild type data, suggesting that we may have identified general drivers of laccase stability. Several sites near Cu, notably 79, 241, and 245, or near substrate, mainly 265, are identified that contribute to stability-function trade-offs, of relevance to the search for new proficient and stable variants of these important industrial enzymes.

General Information

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Organisations: Department of Chemistry, Physical and Biophysical Chemistry
Authors: Christensen, N. J. (Intern), Kepp, K. P. (Intern)
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Stannylene-Mediated Regioselective 6-O-Glycosylation of Unprotected Phenyl 1-Thioglycopyranosides

A straightforward procedure is described for the synthesis of (1→6)-linked saccharides by regioselective glycosylation of unprotected glycosyl acceptors. Phenyl 1-thioglycopyranosides derived from D-glucose, D-galactose and D-mannose were treated with dibutyltin oxide to introduce a stannylene acetal, and then subjected to selective glycosylation at the 6-position with the Koenigs–Knorr protocol. Peracylated glycosyl bromides of D-glucose, D-galactose, D-mannose and D-glucosamine were employed as the donors to give the corresponding (1→6)-linked disaccharides in moderate to good yields. The best results were obtained with glycosyl donors and acceptors derived from D-glucose and D-galactose. Fully acylated disaccharide thioglycosides could also serve as glycosyl donors for the regioselective coupling. Brominolysis and subsequent Koenigs–Knorr coupling with the stannylene acetal of phenyl 1-thio-β-D-glucopyranoside gave rise to the
Structural Characterization of 1,1,3,3-Tetramethylguanidinium Chloride Ionic Liquid by Reversible SO₂ Gas Absorption

A unique new ionic liquid–gas adduct solid state compound formed between 1,1,3,3-tetramethylguanidinium chloride ([tmgH]Cl) and sulfur dioxide has been characterized by X-ray diffraction and Raman spectroscopy. The structure contains SO₂ molecules of near normal structure kept at their positions by Cl–S interactions. The crystals belong in the orthorhombic system, space group Pbcn, with unit cell dimensions of a = 15.6908(10) Å, b = 9.3865(6) Å, and c = 14.1494(9) Å, angles α = β = γ = 90°, and Z = 8 at 120 K. The [tmgH]Cl has a very high absorption capacity of nearly 3 mol of SO₂ per mol of [tmgH]Cl at 1 bar of SO₂ and at room temperature. However, part of the absorbed SO₂ was liberated during the crystallization, probably because the crystal only accommodates one molecule of SO₂ per [tmgH]Cl. The nature of the high absorption capacity of [tmgH]Cl as well as of the homologous compounds with bromide and iodide are discussed. Some of these salts may prove useful as reversible absorbents of SO₂ in industrial flue gases.

General information
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Organisations: Department of Chemistry, X-ray Crystallography, Centre for Catalysis and Sustainable Chemistry
Authors: Berg, R. W. (Intern), Harris, P. (Intern), Riisager, A. (Intern), Fehrmann, R. (Intern)
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Scopus rating (2016): CiteScore 2.64
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 1
Scopus rating (2015): CiteScore 2.78
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 1
Scopus rating (2014): CiteScore 2.65
Web of Science (2014): Indexed yes
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Scopus rating (2013): CiteScore 2.84
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
Study on the Application of the Tie-Line-Table-Look-Up-Based Methods to Flash Calculations in Compositional Simulations

Flash calculation can be a time-consuming part in compositional reservoir simulations, and several approaches have been proposed to speed it up. One recent approach is the shadow-region method that reduces the computation time mainly by skipping stability analysis for a large portion of the compositions in the single-phase region. In the two-phase region, a highly efficient Newton-Raphson algorithm can be used with the initial estimates from the previous step. Another approach is the compositional-space adaptive-tabulation (CSAT) approach, which is based on tie-line table look-up (TTL). It saves computation time by replacing rigorous phase-equilibrium calculations with the stored results in a tie-line table whenever the new feed composition is on one of the stored tie-lines within a certain tolerance. In this study, a modified version of CSAT, named the TTL method, has been proposed to investigate if approximation by looking up a tie-line table can save flash-computation time in the two-phase region. The number of tie-lines stored for comparison and the tolerance set for accepting the feed composition are the key parameters in this method because they will influence the simulation speed and the accuracy of simulation results. We also proposed the tie-line distance-based approximation (TDBA) method, an alternative method to TTL, to obtain approximate flash results in the two-phase region. The method uses the distance to a previous tie-line in the same grid-block to determine whether the approximation should be made. Comparison between the shadow-region approach and the approximation approach, including TTL and TDBA, has been made with a slimtube simulator by which the simulation temperature and the simulation pressure are set constant. It is shown that TDBA can significantly improve the speed in the two-phase region. In contrast, TTL, even with a precalculated tie-line table, is not so advantageous compared with an efficient implementation of rigorous flash. Furthermore, we implemented TDBA in a compositional streamline simulator to apply TDBA to scenarios with pressure variation across the reservoir. We also discussed how to extend TDBA to the general situation in which pressures in grid-blocks are updated dynamically.
Sustained frictional instabilities on nanodomed surfaces: Stick-slip amplitude coefficient

Understanding the frictional properties of nanostructured surfaces is important because of their increasing application in modern miniaturized devices. In this work, lateral force microscopy was used to study the frictional properties between an AFM nanotip and surfaces bearing well-defined nanodomes comprising densely packed prolate spheroids, of diameters ranging from tens to hundreds of nanometers. Our results show that the average lateral force varied linearly with applied load, as described by Amontons' first law of friction, although no direct correlation between the sample topographic properties and their measured friction coefficients was identified. Furthermore, all the nanodomed textures exhibited pronounced oscillations in the shear traces, similar to the classic stick-slip behavior, under all the shear velocities and load regimes studied. That is, the nanotextured topography led to sustained frictional instabilities, effectively with no contact frictional sliding. The amplitude of the stick-slip oscillations, σf, was found to correlate with the topographic properties of the surfaces and scale linearly with the applied load. In line with the friction coefficient, we define the slope of this linear plot as the stick-slip amplitude coefficient (SSAC). We suggest that such stick-slip behaviors are characteristics of surfaces with nanotextures and that such local frictional instabilities have important implications to surface damage and wear. We thus propose that the shear characteristics of the nanodomed surfaces cannot be fully described by the framework of Amontons' laws of friction and that additional parameters (e.g., σf and SSAC) are required, when their friction, lubrication, and wear properties are important considerations in related nanodevices. © 2013 American Chemical Society.
Synthesis and biological evaluation of triazole-containing N-acyl homoserine lactones as quorum sensing modulators

Many bacterial species are capable of assessing their local population densities through a cell–cell signaling mechanism termed quorum sensing (QS). This intercellular communication process is mediated by small molecule or peptide ligands and their cognate protein receptors. Numerous pathogens use QS to initiate virulence once they achieve a threshold cell number on a host. Consequently, approaches to intercept QS have attracted considerable attention as potential anti-infective therapies. Our interest in the development of small molecule tools to modulate QS pathways motivated us to evaluate triazole-containing analogs of natural N-acyl l-homoserine lactone (AHL) signals as non-native QS agonists and antagonists in Gram-negative bacteria. We synthesized 72 triazole derivatives of five broad structure types in high yields and purities using efficient Cu(i)-catalyzed azide–alkyne couplings. These compounds were evaluated for their ability to activate or inhibit two QS receptors from two prevalent pathogens – LasR from Pseudomonas aeruginosa and AbaR from Acinetobacter baumannii – using bacterial reporter strains. Several triazole derivatives were identified that were capable of strongly modulating the activity of LasR and AbaR. These compounds represent a new and synthetically accessible class of AHL analogs, and could find utility as chemical tools to study QS and its role in bacterial virulence.
Synthesis of a Backbone Hexasaccharide Fragment of the Pectic Polysaccharide Rhamnogalacturonan I

Synthesis of the fully unprotected hexasaccharide backbone of the pectic polysaccharide rhamnogalacturonan I is described. The strategy relies on iterative coupling of a common pentenyl disaccharide glycosyl donor followed by a late-stage oxidation of the C-6 positions of the galactose residues. The disaccharide donor is prepared by an efficient chemoselective armed-disarmed coupling of a thiophenyl rhamnoside donor with a pentenyl galactoside acceptor bearing the strongly electron-withdrawing pentafluorobenzoyl ester (PFBz) protective group.

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Authors: Zakharova, A. N. (Intern), Madsen, R. (Intern), Clausen, M. H. (Intern)
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Web of Science (2017): Indexed Yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 6.32 SJR 2.964 SNIP 1.218
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 3.055 SNIP 1.336 CiteScore 6.38
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.958 SNIP 1.324 CiteScore 6.18
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 3.144 SNIP 1.329 CiteScore 6.12
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 3.312 SNIP 1.355 CiteScore 5.7
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 3.271 SNIP 1.377 CiteScore 5.81
ISI indexed (2011): ISI indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 2.985 SNIP 1.307
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 3.048 SNIP 1.37
BFI (2008): BFI-level 2
Scopus rating (2008): SJR 3.263 SNIP 1.295
Web of Science (2008): Indexed yes
Scopus rating (2007): SJR 3.185 SNIP 1.296
Scopus rating (2006): SJR 2.936 SNIP 1.352
Web of Science (2006): Indexed yes
Scopus rating (2005): SJR 2.552 SNIP 1.329
Web of Science (2005): Indexed yes
Scopus rating (2004): SJR 2.515 SNIP 1.262
Web of Science (2004): Indexed yes
Scopus rating (2003): SJR 2.451 SNIP 1.325
Web of Science (2003): Indexed yes
Scopus rating (2002): SJR 2.787 SNIP 1.311
Web of Science (2002): Indexed yes
Scopus rating (2001): SJR 2.266 SNIP 1.427
Web of Science (2001): Indexed yes
Scopus rating (2000): SJR 1.893 SNIP 1.206
Web of Science (2000): Indexed yes
Original language: English
DOIs:
10.1021/ol400430p
Source: dtu
Synthesis of an Orthogonal Topological Analogue of Helicene

The synthesis of an orthogonal topological pentamer analogue of helicene is presented. This analogue forms a tubular structure with its aromatic systems directed parallel to the axis of propagation, which creates a cavity with the potential to function as a host molecule. The synthetic strategy reported, based on a series of repeating Friedländer condensations that utilize pyrido[3,2-d]pyrimidine moieties as protected amino aldehydes, allows for the facile access of higher generations of helical, tubular structures. As a result of the synthetic strategy, only a helical isomer of the pentamer is possible. The structure and absolute configuration of the pentamer were elucidated from a combination of NMR spectroscopic data, optical properties, X-ray structures, and by comparison of an experimental electronic circular dichroism spectrum to a calculated spectrum.

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry, Lund University
Authors: Wixe, T. (Ekstern), Wallentin, C. (Ekstern), Johnson, M. T. (Ekstern), Fristrup, P. (Intern), Lidin, S. (Ekstern), Wärnmark, K. (Ekstern)
Pages: 14963-14969
Publication date: 2013
Main Research Area: Technical/natural sciences

Publication information
Journal: Chemistry: A European Journal
Volume: 19
Issue number: 44
ISSN (Print): 0947-6539
Ratings:
BFI (2018): BFI-level 2
Web of Science (2018): Indexed yes
BFI (2017): BFI-level 2
Web of Science (2017): Indexed yes
BFI (2016): BFI-level 2
Scopus rating (2016): CiteScore 5.03 SJR 2.247 SNIP 1.046
Web of Science (2016): Indexed yes
BFI (2015): BFI-level 2
Scopus rating (2015): SJR 2.416 SNIP 1.184 CiteScore 4.99
Web of Science (2015): Indexed yes
BFI (2014): BFI-level 2
Scopus rating (2014): SJR 2.487 SNIP 1.219 CiteScore 5.51
Web of Science (2014): Indexed yes
BFI (2013): BFI-level 2
Scopus rating (2013): SJR 2.604 SNIP 1.239 CiteScore 5.68
ISI indexed (2013): ISI indexed yes
Web of Science (2013): Indexed yes
BFI (2012): BFI-level 2
Scopus rating (2012): SJR 2.884 SNIP 1.294 CiteScore 5.55
ISI indexed (2012): ISI indexed yes
Web of Science (2012): Indexed yes
BFI (2011): BFI-level 2
Scopus rating (2011): SJR 2.726 SNIP 1.336 CiteScore 5.46
ISI indexed (2011): ISI indexed yes
Web of Science (2011): Indexed yes
BFI (2010): BFI-level 2
Scopus rating (2010): SJR 2.527 SNIP 1.292
Web of Science (2010): Indexed yes
BFI (2009): BFI-level 2
Scopus rating (2009): SJR 2.499 SNIP 1.365
Synthesis of heterocycles through ruthenium-catalyzed ring-closing metathesis and isomerization reactions

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry
Publication date: 2013
Conference: 245th National Spring Meeting of the American-Chemical-Society, New Orleans, LA, United States, 07/04/2013 - 07/04/2013
Main Research Area: Technical/natural sciences

Publication information
Journal: Abstracts of Papers of the American Chemical Society
Volume: 245
Article number: 327
ISSN (Print): 0065-7727

Ratings:
Web of Science (2018): Indexed yes
Web of Science (2017): Indexed Yes
Scopus rating (2014): SJR 0.101 SNIP 0.013
Web of Science (2014): Indexed yes
Scopus rating (2013): SJR 0.101 SNIP 0.003
Web of Science (2013): Indexed yes
Scopus rating (2012): SJR 0.1 SNIP 0
Scopus rating (2011): SJR 0.101 SNIP 0
Web of Science (2011): Indexed yes
Scopus rating (2010): SJR 0.101 SNIP 0
Scopus rating (2009): SJR 0.101 SNIP 0
Synthesis of Human Milk Oligosaccharides and Regioselective Ring Opening of Oxabicycles

This thesis involves two distinct topics related to carbohydrate and organometallic chemistry. The first chapter includes chemical synthesis of oligosaccharides present in human milk. Human milk oligosaccharides are a family of structurally diverse glycans, which are highly unique for human milk. These oligosaccharides participate in multiple mechanisms by which breast-fed infants become protected against infections and they are believed to serve as nutrients for the early brain development. The synthesized oligosaccharides are based on the motif Gal\textsubscript{1–3/4}Glc\textsubscript{NAc}1–3Gal\textsubscript{1–4}Glc, which is the core of many human milk oligosaccharides. Three distinct human milk oligosaccharides were synthesized: Lacto-N-tetraose, Lacto-N-fucopentaose I and Lacto-N-neofucopentaose I. A one-pot strategy was developed for the synthesis of the tetrasaccharide backbone core based on the different reactivity of thioglycoside donors and acceptors. The tetrasaccharides were formed both by sequential and the developed one-pot method. Deprotection of the protecting group at the C-2-position on the galactose moiety liberated an acceptor for the fucosylation eventually creating the two linear pentasaccharides Lacto-N-fucopentaose I and Lacto-N-neofucopentaose I. The scope of the developed one-pot method was further enhanced by performing selective 1-4 glucosylations utilizing a glucosamine building block containing two free hydroxy groups. Furthermore, this work was executed in the hope to synthesize the branched oligosaccharide Lacto-N-fucopentaose III where the fucose is also attached in the same pot. In addition, pNP-neuraminic acid was synthesized for the purpose to perform activity studies on enzymes. The enzymes were designed to perform sialyl transfer reactions in the synthesis human milk oligosaccharides containing neuraminic acid. OH O HO HO O OH O OH O OH O OH O OH OH OH HAc OH O O O HO HO O HOOH OH Lacto-N-fucopentaose OH O HO HO O OH O HO O HO OH O O OH HO HAc Lacto-N-neofucopentaose OH O O HO HO O HOOH OH The second chapter describes the regioselective ring opening of enantiopure oxabicycles primarily by the use of rhodium catalysts and phosphine ligands. The ring opened iii products were similar to compounds, which had shown to be potential protein Bcl-XL antagonists, a target for future drugs in cancer treatment. The aim was to create a general asymmetric ring opening method of several enantiopure oxabicycles having different functional moieties attached to the ring. By employing a [Rh(COD)Cl]\textsubscript{2} catalyst with a Josiphos ligand, it was possible to perform the ring opening of oxabicycles with ester moieties in good yield and excellent regioselectivity. Other functional groups showed to be more challenging, therefore several alterations of the functional groups were performed to form oxabicycles, which could be ring opened regioselectively by the [Rh(COD)Cl]\textsubscript{2} catalyst and Josiphos ligand.

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry
Authors: Jennum, C. A. (Intern), Madsen, R. (Intern)
Number of pages: 158
Publication date: 2013

Publication information
Publisher: DTU Chemistry
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
Source: PublicationPreSubmission
Source-ID: 105128935
Synthesis of Oligosaccharide Fragments of the Pectic Polysaccharide Rhamnogalacturonan I

Pectin is a highly heterogeneous polysaccharide of plant origin. It is found in the primary cell wall and contributes to various cell functions, including support, defense, signaling, and cell adhesion. Pectin also plays an important role as a food additive, serving as a stabilizing and thickening agent in products such as jams, yoghurts, and jellies. Rhamnogalacturonan I is one of the structural classes of pectic polysaccharides, along with homogalacturonan and rhamnogalacturonan II. The chemical structure of rhamnogalacturonan I is complex, having a backbone consisting of alternating L-rhamnose and D-galacturonic acid units with numerous branches of arabinans, galactans, or arabinogalactans positioned at C-4 of the rhamnose residues. The structural complexity of pectin together with the wide range of its practical applications and a desire to understand its structure and functions in detail have inspired many researchers to pursue chemical syntheses of pectic oligosaccharides. Herein, the strategies for chemical synthesis of linear and branched oligosaccharide fragments of rhamnogalacturonan I are presented. The first successful synthesis of a fully unprotected linear hexasaccharide fragment of the rhamnogalacturonan I backbone has been accomplished. The strategy employs a highly modular approach that takes advantage of the armed-disarmed effect to generate the key n-pentenyl disaccharide donor in a chemoselective fashion. Two protected n-pentenyl tetrasaccharide intermediates bearing the digalactan and the diarabinan side-chains have been synthesized. The suitably protected mono- and disaccharide donors have been utilized in the chemoselective glycosylations. The protective group pattern is designed to allow the assembly of larger branched rhamnogalacturonan I fragments.

General information
State: Published
Organisations: Department of Chemistry, Organic Chemistry
Authors: Zakharova, A. (Intern), Clausen, M. H. (Intern), Madsen, R. (Intern)
Number of pages: 118
Publication date: 2013

Publication information
Publisher: Technical University of Denmark, Department of Chemical Engineering
Original language: English
Main Research Area: Technical/natural sciences
Electronic versions:
10-00449-32 Zakharova_Thesis.pdf 1636143_1_1.pdf
Source: dtu
Source-ID: u::8669
Publication: Research › Ph.D. thesis – Annual report year: 2013

Projects:

Experimental investigation of gas injection processes for enhanced oil recovery
Department of Chemistry
Period: 15/03/2018 → 14/03/2021
Number of participants: 4
Phd Student:
Tagliaferri, Stefano (Intern)
Supervisor:
Shapiro, Alexander (Intern)
Yan, Wei (Intern)
Main Supervisor:
Nielsen, Sidsel Marie (Intern)

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

Designing Covalent and Metal-Organic Framework Nanomaterials for Photoelectrochemical Catalysis and Solar Energy Conversion
Department of Chemistry
Period: 01/01/2018 → 31/12/2020
Number of participants: 3
Phd Student:
Pan, Qinying (Intern)
Supervisor:
Tanner, David Ackland (Intern)
Main Supervisor:
Chi, Qijin (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Stipendie fra udlandet
Project: PhD

**Experimental Studies of Polymer Bruch Layers**
Department of Chemistry
Period: 01/01/2018 → 31/12/2020
Number of participants: 3
Phd Student:
Ehtiati, Koosha (Intern)
Supervisor:
Daugaard, Anders Egede (Intern)
Main Supervisor:
Thormann, Esben (Intern)

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

**Graphene supported transition metal oxide composites as metal-ion battery electrode materials**
Department of Chemistry
Period: 01/01/2018 → 31/12/2020
Number of participants: 4
Phd Student:
cao, Huili (Intern)
Supervisor:
Mossin, Susanne (Intern)
Norby, Poul (Intern)
Main Supervisor:
Chi, Qijin (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Stipendie fra udlandet
Project: PhD

**Radiochemical Analysis of Hard-to-measure Radionuclides for Decommissioning and Environmental Trace Studies**
Department of Chemistry
Period: 01/12/2017 → 30/11/2020
Number of participants: 3
Phd Student:
Zhu, Liuchao (Intern)
Supervisor:
Qiao, Jixin (Intern)
Main Supervisor:
Hou, Xiaolin (Intern)

**Financing sources**
Metal centres for activation of small molecules in porous materials

Department of Chemistry
Period: 15/11/2017 → 14/11/2020
Number of participants: 3
PhD Student:
Nielsen, David (Intern)
Supervisor:
Fehrmann, Rasmus (Intern)
Main Supervisor:
Mossin, Susanne (Intern)

Detection and control of bimolecular reactions from preformed weakly bound clusters

Department of Chemistry
Period: 01/11/2017 → 31/10/2020
Number of participants: 4
PhD Student:
Voute, Alexandre Paolo (Intern)
Supervisor:
Larsen, René Wugt (Intern)
Møller, Klaus Braagaard (Intern)
Main Supervisor:
Henriksen, Niels Engholm (Intern)

Design and Engineering of Nanostructured Halide Perovskites for Light Harvesting and Solar Power Conversion

Department of Chemistry
Period: 15/10/2017 → 14/10/2020
Number of participants: 3
PhD Student:
Liang, mingli (Intern)
Supervisor:
Duus, Jens Øllgaard (Intern)
Main Supervisor:
Chi, Qijin (Intern)

Novel Tools for Ultra-Specific Targeting of Nucleic Acids

Department of Chemistry
Period: 15/10/2017 → 14/04/2019
Number of participants: 3
PhD Student:
Faster and Better Structure Determination of Bacterial Polysaccharides for Improved Diagnosis and Vaccines

Department of Chemistry
Period: 01/10/2017 → 30/09/2020
Number of participants: 3
Phd Student:
Li, Chengxin (Intern)
Supervisor:
Gotfredsen, Charlotte Held (Intern)
Main Supervisor:
Duus, Jens Øllgaard (Intern)

Faster and Better Structure Determination of Bacterial Polysaccharides for Improved Diagnosis and Vaccines

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

Novel Response Methods for Challenging Phenomena

Department of Chemistry
Period: 15/09/2017 → 14/09/2020
Number of participants: 3
Phd Student:
Lopez Vidal, Marta (Intern)
Supervisor:
Møller, Klaus Braagaard (Intern)
Main Supervisor:
Coriani, Sonia (Intern)

Novel Response Methods for Challenging Phenomena

Financing sources
Source: Internal funding (public)
Name of research programme: Stipendie fra udlandet
Project: PhD

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)

Design of heterogeneous metal catalysts for C-H Functionalization

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD
Development of polymer-particle composites for adhesive formulations with controlled water uptake kinetics

Department of Chemistry
Period: 01/09/2017 → 31/08/2020
Number of participants: 4
Phd Student:
Eiler, Johannes (Intern)
Supervisor:
Almdal, Kristoffer (Intern)
Bingöl, Bahar (Ekstern)
Main Supervisor:
Thormann, Esben (Intern)

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

Metal-organic frameworks derived non-noble metal caalysts for proton exchange membrane fuel cells

Department of Chemistry
Period: 01/09/2017 → 31/08/2020
Number of participants: 4
Phd Student:
Huang, Wei (Intern)
Supervisor:
Mølhave, Kristian (Intern)
Sun, Hongyu (Intern)
Main Supervisor:
Zhang, Jingdong (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Stipendie fra udlandet
Project: PhD

Development of substantive topicals with high sweat resistance

Department of Chemistry
Period: 15/08/2017 → 14/08/2020
Number of participants: 4
Phd Student:
Keshavarzi, Fatemeh (Intern)
Supervisor:
Jafarzadeh, Shadi (Ekstern)
Lauemøller, Sanne Lise (Ekstern)
Main Supervisor:
Thormann, Esben (Intern)

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

Advancing 2D Materials by Metal-Organic Framework Engineering

Department of Chemistry
Period: 01/08/2017 → 31/07/2020
Number of participants: 3
Phd Student:
Voigt, Laura (Intern)
Supervisor:
Mossin, Susanne (Intern)
Main Supervisor:
Pedersen, Kasper Steen (Intern)

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

Development of polymer skin adhesives with a controlled moisture and sweat removal capacity
Department of Chemistry
Period: 01/06/2017 → 31/05/2020
Number of participants: 4
Phd Student:
Hansen, Daniel (Intern)
Supervisor:
Almdal, Kristoffer (Intern)
Hansen, Kristoffer Karsten (Intern)
Main Supervisor:
Thormann, Esben (Intern)

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

Allosteric regulation of tryptophan hydroxylase isoform 2
Department of Chemistry
Period: 01/05/2017 → 30/04/2020
Number of participants: 4
Phd Student:
Skawinska, Natalia Teresa (Intern)
Supervisor:
Christensen, Hans Erik Mølager (Intern)
Harris, Pernille (Intern)
Main Supervisor:
Peters, Günther H.J. (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
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
Characterization of protein solution structure using light scattering techniques and SAXS

Department of Chemistry
Period: 01/04/2017 → 31/03/2020
Number of participants: 4
Phd Student:
Pohl, Christin (Intern)
Supervisor:
Nørgaard, Allan (Intern)
Peters, Günther H.J. (Intern)
Main Supervisor:
Harris, Pernille (Intern)

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

Metal-Catalyzed Dehydrogenation of Alcohols

Department of Chemistry
Period: 01/04/2017 → 31/03/2020
Number of participants: 3
Phd Student:
Samuelsen, Simone Vestermann (Intern)
Supervisor:
Clausen, Mads Hartvig (Intern)
Main Supervisor:
Madsen, Robert (Intern)

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

Studies of Polynuclear Clusters for Biomass Conversion

Department of Chemistry
Centre for Catalysis and Sustainable Chemistry

Organic Chemistry
Period: 01/03/2017 → 31/08/2017
Number of participants: 1
Project ID: 12-134779
Project participant:
Nielsen, Martin (Intern)

Biomimetic and responsive adhesives for a challenging biological environment

Department of Chemistry
Period: 01/03/2017 → 29/02/2020
Number of participants: 3
Phd Student:
Jiang, Tao (Intern)
Supervisor:
Almdal, Kristoffer (Intern)
Main Supervisor:
Thormann, Esben (Intern)

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

Development of 3-dimensional Graphene Biocatalysts for Enzymatic Biofuel Cells

Department of Chemistry
Period: 01/03/2017 → 29/02/2020
Number of participants: 3
Phd Student:
Tang, Jing (Intern)
Supervisor:
Engelbrekt, Christian (Intern)
Main Supervisor:
Zhang, Jingdong (Intern)

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

High Pressure Phase Behavior of Asymmetric Mixtures for Oil Production

Department of Chemistry  
Period: 01/02/2017 → 31/01/2020  
Number of participants: 4  
Phd Student:  
Liu, Yiqun (Intern)  
Supervisor:  
Regueira Muñiz, Teresa (Intern)  
Stenby, Erling Halfdan (Intern)  
Main Supervisor:  
Yan, Wei (Intern)  

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

Investigations of Compositions and Fluid-Fluid Association Mechanisms for Petroleum Fluids

Department of Chemistry  
Period: 01/02/2017 → 31/01/2020  
Number of participants: 4  
Phd Student:  
Mihrin, Dmytro (Intern)  
Supervisor:  
Henriksen, Jonas Rosager (Intern)  
Larsen, René Wugt (Intern)  
Main Supervisor:  
Feilberg, Karen Louise (Intern)  

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

ALLEVIATE - A novel strategy for food allergy prevention and treatment

Food allergy is an adverse effect to otherwise harmless proteins in the food, whereas oral tolerance is the default result from ingestion of food proteins. Food allergy is a major health problem of growing concern, affecting ~5-8% of young children and 2-4% of adults. No reliable strategy exists for prevention and treatment of food allergy, and strict avoidance of the offending food is presently the only viable management option. Living with food avoidance has a huge impact on the quality of life of food allergic patients, with daily fear of serious or even fatal reactions. The need for efficient methods for prevention and treatment is therefore evident and urgent.  
The purpose of the project is to develop methods to prevent and treat food allergy using a novel strategy, recently invented. Our vision is to overcome limitations in current strategies for food allergy prevention and treatment; being efficient without inducing allergic reactions.
The specific goals of the project are:
1) To develop protein ingredients for a new generation of hypoallergenic (HA) infant formulas (IF) for cow's milk allergy (CMA) prevention
2) To develop a drug candidate for use in immunotherapy (IT) for peanut allergy (PA) treatment

These products would have the capacity to enhance the quality of life for millions of patients in risk of developing CMA and of patients with an already established PA. The market potential is great for both product categories. In addition, the newly developed strategy may form the basis for prevention, treatment and diagnostic products targeting other food allergies.

National Food Institute
Research Group for Gut Microbiology and Immunology
Department of Chemistry
Organic Chemistry
Research Group for Microbial Biotechnology and Biorefining
Office for Innovation & Sector Services
Medical University of Vienna
University of Toronto
University of Leeds
Arla Foods Ingredients Group P/S
Period: 01/01/2017 → 31/12/2020
Number of participants: 7
Food Allergy, Immunotherapy, Infant formula, Allergy, Milk allergy, Peanut allergy
Acronym: ALLEVIATE
Project participant:
Madsen, Charlotte Bernhard (Intern)
Kryger, Karsten (Intern)
Qvortrup, Katrine (Intern)
Jensen, Peter Ruhdal (Intern)
Bang-Berthelsen, Claus Heiner (Intern)
Hulgaard, Egil (Intern)
Project Manager, academic:
Bøgh, Katrine Lindholm (Intern)

Development of Novel Anti-Cancer Drugs using Fragment-Based Drug Discovery
Department of Chemistry
Period: 01/01/2017 → 31/12/2019
Number of participants: 3
Phd Student:
Andersen, Nikolaj Sten (Intern)
Supervisor:
Gottfredsen, Charlotte Held (Intern)
Main Supervisor:
Clausen, Mads Hartvig (Intern)
Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Analysis of reservoir water samples and injected sea water for enhanced oil recovery
Department of Chemistry
Period: 01/11/2016 → 31/10/2019
Number of participants: 3
Phd Student:
Nitsche Gottfredsen, Sofie (Intern)
New approaches to chemical recovery and chelation of underdeveloped radiometals and application of their novel bioconjugates to PET

Department of Chemistry
Period: 01/11/2016 → 31/10/2019
Number of participants: 3
Phd Student: Pedersen, Kristina Søborg (Intern)
Supervisor: Jensen, Mikael (Intern)
Main Supervisor: Zhuravlev, Fedor (Intern)

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)

Metal Catalysts for Dehydrogenation and Decarbonylation of Primary Alcohois

Department of Chemistry
Period: 01/10/2016 → 30/09/2019
Number of participants: 3
Phd Student: Monda, Fabrizio (Ekstern)
Supervisor: Clausen, Mads Hartvig (Intern)
Main Supervisor: Madsen, Robert (Intern)
Metal Catalysts for Dehydrogenation and Decarbonylation of Primary Alcohols

Department of Chemistry
Period: 01/10/2016 → 30/09/2019
Number of participants: 3
PhD Student:
Monda, Fabrizio (Intern)
Supervisor:
Clausen, Mads Hartvig (Intern)
Main Supervisor:
Madsen, Robert (Intern)

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

Tunable and Responsive Properties of Surface Grafted Cross-linked Multilayer Films Containing Alginate Derivatives

Department of Chemistry
Period: 01/10/2016 → 30/09/2019
Number of participants: 3
PhD Student:
Huang, Junhao (Intern)
Supervisor:
Larsen, René Wugt (Intern)
Main Supervisor:
Thormann, Esben (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Stipendie fra udlandet
Project: PhD

Characterisation of Materials based on Graphene and Gold

Department of Chemistry
Period: 01/09/2016 → 31/08/2019
Number of participants: 3
PhD Student:
Nielsen, Frederick Stappen (Intern)
Supervisor:
Engelbrekt, Christian (Intern)
Main Supervisor:
Zhang, Jingdong (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansierede - Virksomhed
Project: PhD

Integrated SILP Catalysts - Membrane Separation Reaction Systems

Department of Chemistry
Period: 01/09/2016 → 31/08/2019
Number of participants: 4
PhD Student:
Marinkovic, Jakob Maximilian (Intern)
Supervisor:
Fehrmann, Rasmus (Intern)
Financing sources
Source: Internal funding (public)
Name of research programme: Anden EU-finansiering
Project: PhD

Long-range interfacial electron transfer between electrode and microorganisms
Department of Chemistry
Period: 15/08/2016 → 14/08/2019
Number of participants: 3
Phd Student:
Zheng, Zhiyong (Intern)
Supervisor:
Christensen, Hans Erik Mølager (Intern)
Main Supervisor:
Zhang, Jingdong (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Stipendie fra udlandet
Project: PhD

Proof of Concept development project for "New low-cost diabetes measuring device".
Department of Chemistry
NanoChemistry
Organic Chemistry
Period: 01/08/2016 → 31/10/2016
Number of participants: 2
Project participant:
Halder, Arnab (Intern)
Chi, Qijin (Intern)

Characterization of protein solution structure using light scattering techniques and SAXS
Department of Chemistry
Period: 01/08/2016 → 31/12/2016
Number of participants: 4
Phd Student:
Mann-Nüttel, Ritu (Intern)
Supervisor:
Nørgaard, Allan (Intern)
Peters, Günther H.J. (Intern)
Main Supervisor:
Harris, Pernille (Intern)

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

Detailed Characterization of weak and strong protein-protein interactions and their structures in concentrated solutions
Department of Chemistry
Structural Biology

Department of Chemistry
Period: 01/08/2016 → 31/07/2019
Number of participants: 4
Phd Student:
Indrakumar, Sowmya (Intern)
Supervisor:
Harris, Pernille (Intern)
Streicher, Werner W. (Ekstern)
Main Supervisor:
Peters, Günther H.J. (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Marie Curie (EU-stipendium)
Project: PhD

Characterization and solution structure of multi-domain proteins and protein complexes

Department of Chemistry
Period: 01/06/2016 → 31/05/2019
Number of participants: 4
Phd Student:
Kulakova, Alina (Intern)
Supervisor:
Due, Anne Vindum (Ekstern)
Peters, Günther H.J. (Intern)
Main Supervisor:
Harris, Pernille (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Marie Curie (EU-stipendium)
Project: PhD

Engineering and structural characterization of perovskite-graphene interfaces for optimizing photovoltaic performance

Department of Chemistry
NanoChemistry
Organic Chemistry
Period: 15/05/2016 → 14/02/2017
Number of participants: 2
Acronym: MAX4ESSFUN
Phd Student:
Halder, Arnab (Intern)  
Project Manager, academic:  
Chi, Qijin (Intern)  
Project

**Development of Zeolite Catalysts and Processes for the Selective Conversion of Sugars to Bio-Polymer Monomers**

Department of Chemistry  
Period: 15/05/2016 → 14/05/2019  
Number of participants: 3  
Phd Student:  
Tosi, Irene (Intern)  
Supervisor:  
Taarning, Esben (Intern)  
Main Supervisor:  
Riisager, Anders (Intern)

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Offentlig finansiering  
Project: PhD

**Development of catalytic reactions to prepare bio-based polymer building blocks**

Department of Chemistry  
Period: 01/05/2016 → 30/04/2019  
Number of participants: 3  
Phd Student:  
Jessen, Bo (Intern)  
Supervisor:  
Taarning, Esben (Intern)  
Main Supervisor:  
Madsen, Robert (Intern)

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Offentlig finansiering  
Project: PhD

**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

**Metal-Catalyzed Dehydrogenation and Decarbonylation of Primary Alcohols**

Department of Chemistry  
Period: 01/05/2016 → 30/04/2019  
Number of participants: 3  
Phd Student:
Stannosilicates in biomass conversion - a combined spectroscopic and computational study

Department of Chemistry  
Period: 01/05/2016 → 30/04/2019  
Number of participants: 3  
PhD Student:  
Elliot, Samuel Gilbert (Intern)  
Supervisor:  
Meier, Sebastian (Intern)  
Main Supervisor:  
Madsen, Robert (Intern)  

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

Protein structure and protein-protein interactions in formulation

Department of Chemistry  
Period: 15/04/2016 → 14/04/2019  
Number of participants: 4  
PhD Student:  
Ryberg, Line Abildgaard (Intern)  
Supervisor:  
Bukrinsky, Jens T. (Ekstern)  
Harris, Pernille (Intern)  
Main Supervisor:  
Peters, Günther H.J. (Intern)  

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

In situ nanoscale investigation of microbial extracellular electron transfer

Department of Chemistry  
NanoChemistry  
Organic Chemistry  
Period: 01/04/2016 → 31/03/2018  
Number of participants: 2  
Supervisor:  
Erik Mølager Christensen, Hans (Ekstern)  
Main Supervisor:  
Zhang, Jingdong (Intern)  
Project
3D Nanocarbon chips for microsupercapacitors and ultrasensitive detection

Department of Chemistry
NanoChemistry
Organic Chemistry
Department of Micro- and Nanotechnology
Period: 15/03/2016 → 14/05/2017
Number of participants: 2
Acronym: CapSens
Phd Student:
Halder, Arnab (Intern)
Hemanth, Suhith (Intern)

Porous Carbon Nanomaterials for Bioelectrochemistry
2-year postdoc project

Department of Chemistry
NanoChemistry
Organic Chemistry
Period: 01/03/2016 → 28/02/2018
Number of participants: 2
Project participant:
Zhao, Jianming (Intern)
Project Coordinator:
Zhang, Jingdong (Intern)

Atomistic Mechanisms of Functional Molecules

Department of Chemistry
Period: 01/02/2016 → 31/01/2019
Number of participants: 4
Phd Student:
Abedi, Mostafa (Intern)
Supervisor:
Henriksen, Niels Engholm (Intern)
Pápai, Mátyás Imre (Intern)
Main Supervisor:
Møller, Klaus Braagaard (Intern)

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

Two-dimensional nanomaterial composites for flexible energy storage and conversion devices

Department of Chemistry
Period: 01/02/2016 → 31/01/2019
Number of participants: 3
Phd Student:
Cao, Xianyi (Intern)
Supervisor:
Chi, Qijin (Intern)
Main Supervisor:
Duus, Jens Øllgaard (Intern)

Financing sources
Development of receptors for Aqueous Carbohydrate Recognition

Department of Chemistry
Period: 01/01/2016 → 31/12/2018
Number of participants: 4
Phd Student:
Baj, Vanessa (Intern)
Supervisor:
Behrens, Carsten (Ekstern)
Nielsen, Thomas Eiland (Intern)
Main Supervisor:
Beeren, Sophie (Intern)

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

Improving Methods for EXAFS studies of Metallo-proteins

Department of Chemistry
Period: 15/12/2015 → 14/12/2019
Number of participants: 3
Phd Student:
Molich, Ulf (Intern)
Supervisor:
Ståhl, Kenny (Intern)
Main Supervisor:
Harris, Pernille (Intern)

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

Nanoscale bioelectrochemistry for development of enzymatic fuel cells

Department of Chemistry
Period: 15/12/2015 → 14/12/2018
Number of participants: 3
Phd Student:
Shen, Fei (Intern)
Supervisor:
Ustrup, Jens (Intern)
Main Supervisor:
Zhang, Jingdong (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme:  Stipendie fra udlandet
Project: PhD

Chemical reactions and intermediates followed by DNP NMR

Department of Chemistry
Period: 01/12/2015 → 30/11/2018
Number of participants: 5
Phd Student:
Boeg, Peter Andreas (Intern)
Supervisor:
Ardenkjær-Larsen, Jan Henrik (Intern)
Duus, Jens Øllgaard (Intern)
Karlsson, Magnus (Ekstern)
Main Supervisor:
Mossin, Susanne (Intern)

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

New Glycosylation Methods for Oligosaccharide Synthesis
Department of Chemistry
Period: 01/12/2015 → 30/11/2018
Number of participants: 3
Phd Student:
Underlin, Emilie Nørmølle (Intern)
Supervisor:
Clausen, Mads Hartvig (Intern)
Main Supervisor:
Madsen, Robert (Intern)

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

Development of Smart Sensor for flow & gas concentration measurement
Center for Bachelor of Engineering Studies
Afdelingen for Informatik
Department of Chemistry
NanoChemistry
Afdelingen for El-teknologi
Donghua University
Period: 01/09/2015 → 31/12/2017
Number of participants: 6
Acronym: SmartSensorFlow
Project ID: 97254
Contact person:
Andersen, Flemming Højskov (Intern)
Project participant:
Hou, Chengyi (Intern)
Sørensen, John Aasted (Intern)
Andersen, Birger (Intern)
Maack, Lars (Intern)
Project Manager, organisational:
Blaszczyk, Tomasz (Intern)

Femtochemistry and Laser Control of Photochemical Reactions
Department of Chemistry
Period: 01/09/2015 → 31/08/2018
Number of participants: 2
Phd Student:
Thomas, Esben Folger (Intern)
Main Supervisor:
Henriksen, Niels Engholm (Intern)

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

Solution structure of Glucagon-peptide 1 analogues and interactions of these peptides with albumin and the endogenous receptor
Department of Chemistry
Period: 01/09/2015 → 31/08/2018
Number of participants: 4
Phd Student:
Frederiksen, Tine Maja (Intern)
Supervisor:
Bukrinsky, Jens T. (Ekstern)
Harris, Pernille (Intern)
Main Supervisor:
Peters, Günther H.J. (Intern)

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

Development of quinones-enriched gold nanoparticles for energy storage and bioelectrochemistry
Department of Chemistry
NanoChemistry
Organic Chemistry
Period: 01/08/2015 → 31/07/2017
Number of participants: 4
Supervisor:
Ulstrup, Jens (Intern)
Tanner, David Ackland (Intern)
Main Supervisor:
Zhang, Jingdong (Intern)
Project Coordinator:
Wagner, Michal (Intern)

Investigation of Bio-nano Materials Produced by Electrochemical Active Bacterial cells at Nanoscale
Department of Chemistry
NanoChemistry
Period: 15/07/2015 → 14/07/2016
Number of participants: 3
Supervisor:
Zhang, Jingdong (Intern)
Ulstrup, Jens (Intern)
Project Coordinator:
Wu, Ranran (Intern)

Project
Transition metal catalysis for synthesis of green, renewable, chemical building blocks

Department of Chemistry
Period: 01/05/2015 → 30/04/2018
Number of participants: 4
Phd Student: Larsen, Daniel Bo (Intern)
Supervisor: Daugaard, Anders Egede (Intern)
Fristrup, Peter (Intern)
Main Supervisor: Duus, Jens Øllgaard (Intern)

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

Ultrafast molecular and X-ray science: Theory and simulations

Department of Chemistry
Period: 01/04/2015 → 18/07/2018
Number of participants: 3
Phd Student: Simmermacher, Mats (Intern)
Supervisor: Henriksen, Niels Engholm (Intern)
Main Supervisor: Møller, Klaus Braagaard (Intern)

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

Three Dimensional Porous Nanoelectrodes for Efficient Energy Conversion

Department of Chemistry
NanoChemistry
Period: 01/01/2015 → 31/12/2015
Number of participants: 1
Project Coordinator: Zhang, Jingdong (Intern)

Electronic properties and surface facet effects of noble metal and semiconductor nanocrystals as catalysts in pure and applied bioelectrochemistry

Department of Chemistry
NanoChemistry
Period: 01/01/2015 → 31/12/2016
Number of participants: 3
Supervisor: Ulstrup, Jens (Intern)
Main Supervisor: Zhang, Jingdong (Intern)
Project Coordinator: Zhang, Ling (Intern)
Chemical Production of 3D Graphene Biocatalysts for Enzymatic Biofuel Cells

Department of Chemistry
NanoChemistry
Period: 01/01/2015 → 31/12/2018
Number of participants: 3
Project participant:
Werchmeister, Rebecka Maria Larsen (Intern)
Shen, Fei (Intern)
Project Coordinator:
Zhang, Jingdong (Intern)

Spectroscopic approaches to understand the catalytic isomerization of carbohydrates

Department of Chemistry
Organic Chemistry
Period: 01/01/2015 → 01/06/2017
Number of participants: 1
Project participant:
Kunov-Kruse, Andreas Jonas (Intern)

Computation of Simultaneous Phase and Chemical Equilibrium

Department of Chemistry
Period: 15/12/2014 → 15/01/2018
Number of participants: 6
Phd Student:
Tsanas, Christos (Intern)
Supervisor:
Stenby, Erling Halfdan (Intern)
Main Supervisor:
Yan, Wei (Intern)
Examiner:
Kontogeorgis, Georgios (Intern)
Jessen, Kristian (Intern)
Solbraa, Even (Ekstern)
Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD

Culticular Polyesters

Department of Chemistry
Period: 15/12/2014 → 14/02/2018
Number of participants: 5
Phd Student:
Martinez San Segundo, Ignacio (Intern)
Main Supervisor:
Clausen, Mads Hartvig (Intern)
Examiner:
Daugaard, Anders Egede (Intern)
Nawrath, Christiane (Ekstern)
Pittelkow, Michael (Ekstern)
Financing sources
Source: Internal funding (public)
**Light-induced electronic and structural dynamics**

Department of Chemistry  
Period: 15/12/2014 → 31/01/2018  
Number of participants: 7  
PhD Student:  
Levi, Gianluca (Intern)  
Supervisor:  
Dohn, Asmus Ougaard (Intern)  
Henriksen, Niels Engholm (Intern)  
Main Supervisor:  
Møller, Klaus Braagaard (Intern)  
Examiner:  
Schiøtz, Jakob (Intern)  
Chergui, Mejed (Ekstern)  
González, Leticia (Ekstern)

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

**Polyesters from Plant Cutin**

Department of Chemistry  
Period: 15/12/2014 → 14/02/2018  
Number of participants: 5  
PhD Student:  
Scavée, Gauthier Mike L (Intern)  
Main Supervisor:  
Clausen, Mads Hartvig (Intern)  
Examiner:  
Woodley, John (Intern)  
J. Minnaard, Adriaan (Ekstern)  
Nielsen, Mogens Brøndsted (Ekstern)

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

**Remote loading strategies for incorporation of therapeutic compounds and contrast agents into gels and liposomes**

Department of Chemistry  
Period: 15/12/2014 → 14/03/2018  
Number of participants: 5  
PhD Student:  
Engudar, Gokce (Intern)  
Supervisor:  
Andresen, Thomas Lars (Intern)  
Jensen, Andreas Tue Ingemann (Intern)  
Thormann, Esben (Intern)  
Main Supervisor:  
Henriksen, Jonas Rosager (Intern)

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Institut stipendie (DTU)
Selective Hydrogenation of 1,3-butadiene
Department of Chemistry
Centre for Catalysis and Sustainable Chemistry
Period: 01/12/2014 → ...
Number of participants: 2
hydrogenation; continuous flow reactions; fixed-bed reactors; palladium; heterogeneous catalysts; metal nanoparticles
Project participant:
Garcia Suárez, Eduardo José (Intern)
Riisager, Anders (Intern)

In Silico Prediction of the Substrate Specificity of Sirtuins in Combination Synthesis and Biochemical Profiling
Department of Chemistry
Period: 01/11/2014 → 14/03/2018
Number of participants: 8
Phd Student:
Colaço, Ana Rita Freitas (Intern)
Supervisor:
Duus, Jens Øllgaard (Intern)
Fristrup, Peter (Intern)
Olsen, Christian Adam (Intern)
Main Supervisor:
Peters, Günther H.J. (Intern)
Examiner:
Kepp, Kasper Planeta (Intern)
Lindorff-Larsen, Kresten (Ekstern)
Sippl, Wolfgang (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansierede - Virksomhed

Development of new NMR methods for the elucidation of carbohydrate converting enzyme mechanisms and optimization of enzyme processes in future green synthesis
Department of Chemistry
Period: 15/10/2014 → 14/03/2018
Number of participants: 5
Phd Student:
Kjeldsen, Christian (Intern)
Main Supervisor:
Duus, Jens Øllgaard (Intern)
Examiner:
Jensen, Pernille Rose (Intern)
Angulo, Jesus (Ekstern)
Larsen, Flemming Hofmann (Ekstern)

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

Metalloproteins in Alzheimer's disease
Department of Chemistry
Period: 15/09/2014 → 24/01/2018
Number of participants: 6
Phd Student: Somavarapu, Arun Kumar (Intern)
Supervisor: Peters, Günther H.J. (Intern)
Main Supervisor: Kepp, Kasper Planeta (Intern)
Examiner: Harris, Pernille (Intern)
Hureau-Sabater, Christelle (Ekstern)
Jensen, Jan Halborg (Ekstern)

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

Compositional Simulation of Heavy Oil Production with Steam and Solvent
Department of Chemistry
Period: 01/09/2014 → 13/12/2017
Number of participants: 7
Phd Student: Paterson, Duncan (Intern)
Supervisor: Michelsen, Michael Locht (Intern)
Stenby, Erling Halfdan (Intern)
Main Supervisor: Yan, Wei (Intern)
Examiner: Henriksen, Niels Engholm (Intern)
Hendriks, Eric Maria (Ekstern)
Montel, François (Ekstern)

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

Structure and function of the regulatory domain in tryptophanhydroxulase
Department of Chemistry
Period: 01/09/2014 → 14/02/2018
Number of participants: 7
Phd Student: Tidemand, Kasper Damgaard (Intern)
Supervisor: Christensen, Hans Erik Mølager (Intern)
Harris, Pernille (Intern)
Main Supervisor: Peters, Günther H.J. (Intern)
Examiner: Duus, Jens Øllgaard (Intern)
Thörölsson, Matthias (Ekstern)
Westh, Peter (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD
Compositional Reservoir Simulation Involving Complex Pase Equilibria

Department of Chemistry
Period: 01/07/2014 → 30/09/2017
Number of participants: 7
Phd Student:
Sandoval Lemus, Diego Rolando (Intern)
Supervisor:
Michelsen, Michael Locht (Intern)
Stenby, Erling Halfdan (Intern)
Main Supervisor:
Yan, Wei (Intern)
Examiner:
Shapiro, Alexander (Intern)
Galliéro, Guillaume (Ekstern)
Koch, Oliver (Ekstern)

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

Relations
Publications:
Phase Equilibrium Modeling for Shale Production Simulation
Project: PhD

Experimental Physical Chemistry of Polymers and Polyelectrolytes

Department of Chemistry
Period: 01/06/2014 → 20/09/2017
Number of participants: 5
Phd Student:
Moghaddam, Saeed Zajforoushan (Intern)
Main Supervisor:
Thormann, Esben (Intern)
Examiner:
Duus, Jens Ølgaard (Intern)
Claesson, Per Martin (Ekstern)
Westh, Peter (Intern)

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

Relations
Publications:
Specific Ion Effects in Thermo-Responsive Polymer Solutions
Project: PhD

Low Temperature deNOx Technologies for Power and Waste Incineration Plants

Department of Chemistry
Period: 01/06/2014 → 30/09/2017
Number of participants: 7
Phd Student:
Petersen, Peter Westergaard (Intern)
Supervisor:
Jensen, Anker Degn (Intern)
Mossin, Susanne (Intern)
Valorisation of lignocellulosic biomass side streams for sustainable production of chemicals, materials & fuels using low environmental impact technologies

Scientists are prompted to seek alternative methodologies for the production of materials, fuels and chemicals using low environmental impact technologies and greener methodologies with comparable efficiencies to those currently available in view of the expected resource scarcity and future oil economy. Lignocellulosic residues can constitute a highly promising (and currently largely under-utilised) feedstock with a significant potential to be converted into useful end products. However, a joint multidisciplinary effort from several disciplines including (bio)chemistry, biology, (bio)chemical and biological engineering, forest products sciences as well as environmental sciences and experts in economic assessment in liaison with industry is required to appropriately address the efficient transformation of such residues. The main objective of this COST Action will be to develop a solid European multidisciplinary network able to provide a range of innovative alternatives to the valorisation of lignocellulosic residues to chemicals, fuels and materials making use of environmentally sound protocols from.

Department of Chemistry
Centre for Catalysis and Sustainable Chemistry

EU COST Office
Period: 14/05/2014 → 13/05/2018
Number of participants: 2
Valorisation of Lignocellulosic Biomass Residues, Forest Products, Biorefinery
Acronym: FP1306
Project ID: FP1306
Project participant:
Garcia Suárez, Eduardo José (Intern)
Riisager, Anders (Intern)
Project

Oxidative catalytic upgrading of carbohydrates and derivatives from biomass

Department of Chemistry
Period: 01/05/2014 → 20/09/2017
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
Relations
Publications:
Selective Oxidation of Biomass-Derived Chemicals
Project: PhD

Synthesis and investigation of prodrugs
Department of Chemistry
Period: 01/05/2014 → 24/01/2018
Number of participants: 5
Phd Student:
Peiro, Jorge (Intern)
Main Supervisor:
Clausen, Mads Hartvig (Intern)
Examiner:
Astakhova, Kira (Intern)
Almqvist, Fredrik (Ekstern)
Olsen, Christian Adam (Intern)

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

Chemical Production of Graphene Catalysts for Electrochemical Energy Conversion
Department of Chemistry
Period: 15/03/2014 → 13/11/2017
Number of participants: 6
Phd Student:
Seselj, Nedjeljko (Intern)
Supervisor:
Ulstrup, Jens (Intern)
Main Supervisor:
Zhang, Jingdong (Intern)
Examiner:
Henriksen, Niels Engholm (Intern)
Nørgaard, Kasper (Ekstern)
Wollenberger, Ulla (Ekstern)

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

Relations
Publications:
Chemical Production of Graphene Catalysts for Electrochemical Energy Conversion
Project: PhD

Studies of Polynuclear Clusters for Biomass Conversion
Department of Chemistry
Centre for Catalysis and Sustainable Chemistry
Organic Chemistry
Period: 01/03/2014 → 28/02/2017
Number of participants: 1
Project ID: 12-131997
Project participant:
Nielsen, Martin (Intern)
Project
Studies of Polynuclear Clusters for Biomass Conversion
Department of Chemistry
Centre for Catalysis and Sustainable Chemistry
Organic Chemistry
Period: 01/01/2014 → 31/12/2015
Number of participants: 1
Acronym: STUPOSTERMAC
Project participant:
Nielsen, Martin (Intern)

Chemical Production of Graphene Catalysts for Electrochemical Energy Conversion
Department of Chemistry
NanoChemistry
Period: 01/01/2014 → 31/12/2016
Number of participants: 2
Project participant:
Seselj, Nedjeljko (Intern)
Project Coordinator:
Zhang, Jingdong (Intern)

Functional gold-based nanomaterials
Department of Chemistry
NanoChemistry
Period: 01/01/2014 → 31/12/2015
Number of participants: 1
Project Coordinator:
Zhang, Jingdong (Intern)

Noble Metals Free Intermediate -Temperature Supported Liquid Phase Electrolyzer
The strategic development of the NobleFree project is noble metal free intermediate-temperature (200-400 C) fuel cells and water electrolyser with the same characteristics as of the Nafto®, PBI and Aquivion™ systems. This goal will be achieved by use of alkaline metals dihydrogen phosphates as proton-conducting supported liquid phase electrolytes (SLPE). These electrolytes will be liquid immobilized on ceramic nano fibers, whiskers and powders. It has been discovered recently, that nickel, high-nickel alloys and austenitic stainless steels containing small amounts of Ti have high corrosion resistance in the molten alkali metals dihydrogen phosphates in the above mentioned temperature range. The NobleFree will start with the parallel development of electrolytes and nickel-based catalysts. The final stage of the project will be design and test of noble metal free intermediate temperature water electrolyser. Possibilities of use SLPE system as a fuel cell will be also studied.
Department of Energy Conversion and Storage
Proton conductors
Energy and Materials
Period: 01/01/2014 → ...
Number of participants: 5
Acronym: Noble Free
Project participant:
Nikiforov, Aleksey Valerievich (Intern)
Bjerrum, Niels J. (Intern)
Petrushina, Irina (Intern)
Christensen, Erik (Intern)
Jensen, Jens Oluf (Intern)
Study of High Pressure and High Temperature Reservoir Fluids

Department of Chemistry
Period: 15/12/2013 → 25/08/2017
Number of participants: 6
Phd Student:
Varzandeh, Farhad (Intern)
Supervisor:
Stenby, Erling Halfdan (Intern)
Main Supervisor:
Yan, Wei (Intern)
Examiner:
Møller, Klaus Braagaard (Intern)
Lindeloff, Niels (Intern)
Montel, François (Ekstern)

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

Relations
Publications:
Modeling Study of High Pressure and High Temperature Reservoir Fluids
Project: PhD

Effective production of Hydrogen at 200-400 degr. C

Department of Chemistry
Period: 01/12/2013 → 30/11/2014
Number of participants: 1
Hydrogen Energy Raman Spectroscopy
Project participant:
Berg, Rolf W. (Intern)

Nanostructured and Free-standing Grahene Paper Sensors for Ultrasensitive Monitoring of Food Quality and Safety

Department of Chemistry
Period: 01/12/2013 → 26/04/2017
Number of participants: 6
Phd Student:
Zhang, Minwei (Intern)
Supervisor:
Ulstrup, Jens (Intern)
Main Supervisor:
Chi, Qijin (Intern)
Examiner:
Mossin, Susanne (Intern)
Mandler, Daniel (Ekstern)
Nielsen, Mogens Brøndsted (Ekstern)

Financing sources
Synthesis of plant cell wall oligosaccharides

Department of Chemistry
Period: 01/12/2013 → 13/12/2017
Number of participants: 5
Phd Student: Mancuso, Enzo (Intern)
Main Supervisor: Clausen, Mads Hartvig (Intern)
Examiner: Gotfredsen, Charlotte Held (Intern)
Jensen, Henrik Helligsø (Ekstern)
Lowary, Todd L. (Ekstern)

Bioengineering Functionalization of Graphene Nanomaterials for Sensor Applications

Department of Chemistry
Period: 15/11/2013 → 25/08/2017
Number of participants: 6
Phd Student: Halder, Arnab (Intern)
Supervisor: Ulstrup, Jens (Intern)
Main Supervisor: Chi, Qijin (Intern)
Examiner: Duus, Jens Øllgaard (Intern)
Boukherroub, Rabah (Ekstern)
Jensen, Knud Jørgen (Intern)

Mechanistic Investigation of the Manganese-Catalyzed Cross Coupling Reaction

Department of Chemistry
Period: 15/11/2013 → 14/02/2018
Number of participants: 5
Phd Student: Antonacci, Giuseppe (Intern)
Main Supervisor: Madsen, Robert (Intern)
Manganese Catalysts for the Cross Coupling Reaction

Department of Chemistry
Period: 01/11/2013 → 14/03/2018
Number of participants: 5
Phd Student:
Ahlburg, Andreas (Intern)
Main Supervisor:
Madsen, Robert (Intern)
Examiner:
Tanner, David Ackland (Intern)

Nanoporous Chemical Graphene for High-performance Electrocatalytic Energy Conversion
The postdoc project supported by the Hand C. Ørsted Postdoc Program.

Department of Chemistry
NanoChemistry
Period: 01/10/2013 → 30/09/2014
Number of participants: 2
Project participant:
Chi, Qijin (Intern)
Dey, Ramendra Sundar (Intern)

Spectroscopic Investigations of Copper Substituted Zeolite Catalysts

Department of Chemistry
Period: 01/10/2013 → 24/01/2018
Number of participants: 6
Phd Student:
Godiksen, Anita (Intern)
Supervisor:
Rasmussen, Søren Birk (Intern)
Main Supervisor:
Mossin, Susanne (Intern)
Examiner:
Riisager, Anders (Intern)
Chiesa, Mario (Ekstern)
Wang, Feng Ryan (Ekstern)

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

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

Financing sources
Source: Internal funding (public)
Name of research programme: Samfinansierede - Virksomhed
Project: PhD

**Sustainable Chemistry for Biomass Utilization**

Department of Chemistry  
Period: 01/10/2013 → 17/05/2017  
Number of participants: 6  
Phd Student: Nielsen, Lasse Bo (Intern)  
Supervisor: Fristrup, Peter (Intern)  
Main Supervisor: Tanner, David Ackland (Intern)  
Examiner: Riisager, Anders (Intern)  
Moret, Marc-Etienne (Ekstern)  
Pittelkow, Michael (Ekstern)  

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

**Relations**  
Publications:  
Sustainable Chemistry for Biomass Utilization  
Project: PhD

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**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

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**Benign Homogeneous Catalysis with Transition Metals**

Department of Chemistry  
Period: 15/09/2013 → 20/09/2017  
Number of participants: 5  
Phd Student: Santilli, Carola (Intern)  
Main Supervisor: Madsen, Robert (Intern)  
Examiner: Gotfredsen, Charlotte Held (Intern)  
Nielsen, Mogens Brøndsted (Ekstern)  
Wendt, Ola F. (Ekstern)  

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Institut stipendie (DTU)
Relations
Publications:
Transition Metal Catalyzed Synthesis of Carboxylic Acids, Imines, and Biaryls
Project: PhD

In-Bead Diagnostics and Screening
Department of Chemistry
Period: 15/09/2013 → 31/10/2014
Number of participants: 2
Phd Student:
Væring, Philip (Intern)
Main Supervisor:
Nielsen, Thomas Eiland (Intern)

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

Microfabrication an Chemical Functionalization of Tailor-made Materials for Biomedical Applications
Department of Chemistry
Period: 01/09/2013 → 21/06/2017
Number of participants: 6
Phd Student:
Mortensen, Kim Thollund (Intern)
Supervisor:
Nielsen, Thomas Eiland (Intern)
Main Supervisor:
Qvortrup, Katrine (Intern)
Examiner:
Tanner, David Ackland (Intern)
Meldal, Morten (Ekstern)
Spring, David Robert (Ekstern)

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

Relations
Publications:
Development of a UV-Cleavable Protecting Group for Hydroxylamines, Synthesis of a StructurallyWide Variety of Hydroxamic Acids, and Identification of Histone Deacetylase Inhibitors
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.

**Relations**
Publications:
Synthesis, Characterization and Evaluation of Tin-containing Silicates for Biomass Conversion
Project: PhD

**Transition Metal-Catalyzed Carbon-Carbon Bond Transformation**
Department of Chemistry
Period: 01/09/2013 → 14/02/2018
Number of participants: 5
Phd Student:
Mazziotta, Andrea (Intern)
Main Supervisor:
Madsen, Robert (Intern)
Examiner:
Gotfredsen, Charlotte Held (Intern)
Ahlquist, Mårten Sten Güsta (Intern)
Lindhardt, Anders Thyboe (Ekstern)

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

**Bioengineering Functionalization of Chemical Graphenes for Biosensing Devices**
Department of Chemistry
Period: 01/06/2013 → 19/07/2013
Number of participants: 3
Phd Student:
Lin, Qianqian (Intern)
Supervisor:
Ulstrup, Jens (Intern)
Main Supervisor:
Chi, Qijin (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Institut, samfinansiering
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:
Melián 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.

Relations
Publications:
Design of sintering-stable heterogeneous catalysts
Project: PhD

Shedding Light on Macroscopic Systems One Molecule at a Time: Spectroscopy of Organic Hydrogen-Bonded Clusters
Department of Chemistry
Period: 01/05/2013 → 31/08/2016
Number of participants: 3
Phd Student:
Wallin Mahler Andersen, Denise (Intern)
Supervisor:
Larsen, René Wugt (Intern)
Main Supervisor:
Møller, Klaus Braagaard (Intern)

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

Solving the 3D structural Puzzle
Department of Chemistry
Period: 01/05/2013 → 20/09/2016
Number of participants: 5
Phd Student:
Hoeck, Casper (Intern)
Main Supervisor:
Gotfredsen, Charlotte Held (Intern)
Examiner:
Duus, Jens Øllgaard (Intern)
Luy, Burkhard (Ekstern)
Vosegaard, Thomas (Ekstern)

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

Relations
Publications:
Solving a 3D structural puzzle
Project: PhD

Supermolecular Derivation of Graphene Nanomaterials for Chemical Sensors

Department of Chemistry
Period: 01/05/2013 → 18/08/2016
Number of participants: 6
Phd Student:
Olsen, Gunnar (Intern)
Supervisor:
Ulstrup, Jens (Intern)
Main Supervisor:
Chi, Qijin (Intern)
Examiner:
Duus, Jens Øllgaard (Intern)
Gorton, Lo Gunnar Otto (Ekstern)
Nielsen, Mogens Brøndsted (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut, samfinansiering

Relations
Publications:
Supramolecular Derivation of Graphene Nanomaterials for Chemical Sensors
Project: PhD

Structural properties and formulation of hydrophobic peptides

Department of Chemistry
Period: 01/04/2013 → 30/09/2016
Number of participants: 7
Phd Student:
Sanderby, Pernille (Intern)
Supervisor:
Peters, Günther H.J. (Intern)
Peters, Günther H.J. (Intern)
Main Supervisor:
Harris, Pernille (Intern)
Examiner:
Gotfredsen, Charlotte Held (Intern)
 André, Ingemar (Ekstern)
Pedersen, Jan Skov (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU) Samf.
Relations
Publications:
Solution behaviour of Human Serum Albumin and GLP-1 variants
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.

Relations
Publications:
Design of porous nanostructured solid catalysts
Project: PhD

Nanoguide: Development of targeted nanoparticles for improving image-guided radiotherapy
Department of Chemistry
Period: 01/03/2013 → 21/06/2017
Number of participants: 5
Phd Student:
Schaarup-Jensen, Henrik (Intern)
Main Supervisor:
Clausen, Mads Hartvig (Intern)
Examiner:
Urquhart, Andrew (Intern)
Jensen, Knud Jørgen (Intern)
Ovaa, Huib (Ekstern)

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

Relations
Publications:
Synthesis and Development of Diagnostic Tools for Medical Imaging
Project: PhD

Synthesis of algaloligosaccharides
Department of Chemistry
Period: 01/03/2013 → 21/06/2017
Number of participants: 5
Phd Student:
Kinnaert, Christine (Intern)
Main Supervisor:
Clausen, Mads Hartvig (Intern)
Examiner:
Madsen, Robert (Intern)
Jensen, Henrik Helligsø (Ekstern)
Pfrengle, Fabian (Ekstern)

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

Relations
Publications:
Towards the Synthesis of Carrageenan Oligosaccharides
Project: PhD

Oligosaccharide Synthesis with Unprotected Carbohydrates
Department of Chemistry
Period: 01/02/2013 → 14/12/2016
Number of participants: 5
Phd Student:
Niedbal, Dominika (Intern)
Main Supervisor:
Madsen, Robert (Intern)
Examiner:
Tanner, David Ackland (Intern)
Jensen, Henrik Helligsø (Ekstern)
Oscarson, Stefan (Ekstern)

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

Relations
Publications:
Method Development in the Regioselective Glycosylation of Unprotected Carbohydrates
Project: PhD

Metal-Directed Glycosylation with Unprotected Carbohydrates
Department of Chemistry
Period: 15/12/2012 → 20/09/2016
Number of participants: 5
Phd Student:
Lanz, Gyrithe (Intern)
Main Supervisor:
Madsen, Robert (Intern)
Examiner:
Gotfredsen, Charlotte Held (Intern)
Jensen, Henrik Helligsø (Ekstern)
Oscarson, Stefan (Ekstern)

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

Relations
Publications:
Glycosyl Bromides in Glycoside Synthesis: Development of New Promoter System and Metal-Mediated Regioselective Glycosylations
Project: PhD
Chemical Synthesis of Hemicellulose Fragments

Department of Chemistry
Period: 01/12/2012 → 26/10/2016
Number of participants: 5
PhD Student:
Böhm, Maximilian Felix (Intern)
Main Supervisor:
Madsen, Robert (Intern)
Examiner:
Clausen, Mads Hartvig (Intern)
Oscarson, Stefan (Ekstern)
Pedersen, Christian Marcus (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering

Relations
Publications:
Chemical Synthesis of Hemicellulose Fragments
Project: PhD

Kinetic Annotation of Structurally Diverse Lysine Deacylase (KDAC) Inhibitors

Department of Chemistry
Period: 01/11/2012 → 28/02/2014
Number of participants: 2
PhD Student:
Stephansen, Helle Marie (Intern)
Main Supervisor:
Olsen, Christian Adam (Intern)

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

Synthesis of Oligosaccharides related to the plant polysaccharide hemicellulose

Department of Chemistry
Period: 01/11/2012 → 20/04/2016
Number of participants: 5
PhD Student:
Bonora, Beatrice (Intern)
Main Supervisor:
Clausen, Mads Hartvig (Intern)
Examiner:
Gotfredsen, Charlotte Held (Intern)
Jensen, Henrik Helligsø (Ekstern)
Werz, Daniel B. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering

Relations
Publications:
Synthesis of S-linked oligoxylans
Project: PhD
Synthesis of Saccharides related to Plant Cell Wall Carbohydrates

Department of Chemistry
Period: 01/11/2012 → 18/08/2016
Number of participants: 5
Phd Student: d’Errico, Clotilde (Intern)
Main Supervisor: Madsen, Robert (Intern)
Examiner: Duus, Jens Øllgaard (Intern)
Jensen, Henrik Helligse (Ekstern)
Widmalm, Göran (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering

Relations
Publications:
Glucuronic Acid Derivatives in Enzymatic Biomass Degradation: Synthesis and Evaluation of Enzymatic Activity
Project: PhD

Bio-fuel synthesis with solid acid functionalized catalysis

Department of Chemistry
Period: 01/09/2012 → 02/12/2015
Number of participants: 6
Phd Student: Poreddy, Raju (Intern)
Supervisor: Jensen, Anker Degn (Intern)
Main Supervisor: Riisager, Anders (Intern)
Examiner: Ståhl, Kenny (Intern)
Grunwaldt, Jan-Dierk (Intern)
Herbst, Konrad (Ekstern)

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

Spectroscopy of weakly bound solvent-water Cluster molecules

Department of Chemistry
Period: 01/09/2012 → 22/02/2016
Number of participants: 6
Phd Student: Andersen, Jonas (Intern)
Supervisor: Ståhl, Kenny (Intern)
Main Supervisor: Larsen, René Wugt (Intern)
Examiner: Henriksen, Niels Engholm (Intern)
Johnson, Matthew (Ekstern)
Nielsen, Claus Jørgen (Ekstern)
Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)

Relations
Publications:
Far-Infrared Spectroscopy of Weakly Bound Hydrated Cluster Molecules
Project: PhD

Synthesis of thiooligosaccharides related to the plant polysaccharide cellulose
Department of Chemistry
Period: 15/07/2012 → 14/12/2016
Number of participants: 5
Phd Student:
Nami, Faranak (Intern)
Main Supervisor:
Clausen, Mads Hartvig (Intern)
Examiner:
Gotfredsen, Charlotte Held (Intern)
Galan, Carmen (Ekstern)
Werz, Daniel B. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering

Relations
Publications:
Synthesis of S-linked cello-oligosaccharides
Project: PhD

Radicals for dynamic nuclear polarisation
Department of Chemistry
Period: 01/06/2012 → 23/09/2016
Number of participants: 4
Phd Student:
Jensen, Jonas (Intern)
Supervisor:
Ardenkjær-Larsen, Jan Henrik (Intern)
Tanner, David Ackland (Intern)
Main Supervisor:
Mossin, Susanne (Intern)

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

SILP catalysts for alkoxy carbonylation
Department of Chemistry
Centre for Catalysis and Sustainable Chemistry
Period: 01/05/2012 → 30/04/2015
Number of participants: 4
ionic liquids, brensted acid, carbonylation, palladium
Acronym: SILP
Number of related Ph.D. students: 1
Project participant:
Garcia Suárez, Eduardo José (Intern)
Bio-chemicals synthesis with ionic liquid technology

Department of Chemistry
Period: 15/03/2012 → 30/09/2016
Number of participants: 5
PhD Student:
Paolicchi, Dario (Intern)
Main Supervisor:
Riisager, Anders (Intern)
Examiner:
Fehrmann, Rasmus (Intern)
Claver, Carmen (Ekstern)
Vogel, Stefan (Ekstern)

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

Relations
Publications:
Methoxycarbonylation of alkenes with biomass-derived CO
Project: PhD

Ruthenium-Catalyzed Tandem RCM/Isomerization Sequences

Department of Chemistry
Period: 15/03/2012 → 03/06/2015
Number of participants: 6
PhD Student:
Ishøj, Mette (Intern)
Supervisor:
Nielsen, Thomas Eiland (Intern)
Main Supervisor:
Tanner, David Ackland (Intern)
Examiner:
Andresen, Thomas Lars (Intern)
Nelson, Adam S. (Ekstern)
Poulsen, Thomas Bjørn (Intern)

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

**Total synthesis of Sioboldine A**
Department of Chemistry
Period: 15/03/2012 → 02/09/2015
Number of participants: 6
Phd Student:
Olsen, Lasse Bohn (Intern)
Supervisor:
Nielsen, Thomas Eiland (Intern)
Main Supervisor:
Tanner, David Ackland (Intern)
Examiner:
Duus, Jens Øllgaard (Intern)
Craig, Donald (Ekstern)
Nielsen, John (Intern)

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

**Catalysis Orhestration: One Catalysts with multiple modes of Action**
Department of Chemistry
Period: 01/03/2012 → 03/06/2015
Number of participants: 6
Phd Student:
Ohm, Ragnhild Gaard (Intern)
Supervisor:
Nielsen, Thomas Eiland (Intern)
Main Supervisor:
Tanner, David Ackland (Intern)
Examiner:
Fristrup, Peter (Intern)
Andersson, Pher G. (Ekstern)
Nielsen, Mogens Brøndsted (Ekstern)

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

**Sustainable Chemistry for Biomass Utilization**
Department of Chemistry
Period: 15/02/2012 → 30/09/2015
Number of participants: 5
Phd Student:
Lupp, Daniel (Intern)
Investigation of Solid / Liquid Electrochemical Interfaces at Nanometer Scale

Department of Chemistry

NanoChemistry
Period: 01/01/2012 → 31/12/2014
Number of participants: 4
Project participant:
Engelbrekt, Christian (Intern)
Jensen, Palle Skovhus (Intern)
Dey, Ramendra Sundar (Intern)

Project Coordinator:
Zhang, Jingdong (Intern)

Ligand assisted Site-Specific Modification of Proteins

Department of Chemistry
Period: 01/01/2012 → 30/09/2015
Number of participants: 6
Phd Student:
Bang, Claus Gunnar (Intern)
Supervisor:
Nielsen, Thomas Eiland (Intern)
Main Supervisor:
Tanner, David Ackland (Intern)
Examiner:
Gotfredsen, Charlotte Held (Intern)
Heinis, Christian (Ekstern)
Jensen, Knud Jørgen (Intern)

Speciation Analysis and Environmental Tracer Studies of 129I

Department of Chemistry
Period: 15/12/2011 → 02/09/2015
Number of participants: 5
Phd Student:
Zhang, Luyuan (Intern)
Main Supervisor:
Hou, Xiaolin (Intern)
Examiner:
Nielsen, Sven Poul (Intern)
Aldahan, Ala A. (Ekstern)
Baker, Alexander (Ekstern)

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

**High-efficiency, low-cost electrode surfaces for next generation alkaline electrolysis**
Department of Energy Conversion and Storage
Proton conductors
Energy and Materials
Department of Chemistry
Department of Chemistry
Period: 14/12/2011 → 12/12/2014
Number of participants: 3
Alkaline Electrolysis, Water splitting, Electrodes, Sustainable Energy
Project ID: J.nr. 068-2011-1
Project participant:
Nikiforov, Aleksey Valerievich (Intern)
Jensen, Jens Oluf (Intern)
Bjerrum, Niels J. (Intern)

**Academic Excellence Scholarship**
Department of Chemistry
Centre for Catalysis and Sustainable Chemistry
Period: 01/12/2011 → 28/02/2015
Number of participants: 1
Project participant:
Kolding, Helene (Intern)

**Katalyse og selektiv gasabsorption i ioniske væsker**
Department of Chemistry
Period: 01/12/2011 → 03/06/2015
Number of participants: 6
Phd Student:
Kolding, Helene (Intern)
Supervisor:
Riisager, Anders (Intern)
Main Supervisor:
Fehrmann, Rasmus (Intern)
Examiner:
Berg, Rolf W. (Intern)
Dupont, Jairton (Ekstern)
Olsen, Espen (Ekstern)

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

**Sustainable Chemistry for Biomass Utilization**
Department of Chemistry
Biomimetic Foldamers with New Backbone Architectures

Department of Chemistry
Period: 15/11/2011 → 03/06/2015
Number of participants: 6
Phd Student:
Engel-Andreasen, Jens (Intern)
Supervisor:
Olsen, Christian Adam (Intern)
Main Supervisor:
Fristrup, Peter (Intern)
Examiner:
Gotfredsen, Charlotte Held (Intern)
Heeg-Jensen, Thomas (Ekstern)
Maarseveen, Jan Van (Ekstern)

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

Synthesis of Antibacterial Tetrahydro-b-Carbolines via Metal-Catalyzed N-Allylamine Isomerization/N-Alkyliminium Cyclization Sequence

Department of Chemistry
Period: 01/11/2011 → 04/02/2015
Number of participants: 6
Phd Student:
Hansen, Casper Lykke (Intern)
Supervisor:
Nielsen, Thomas Eiland (Intern)
Main Supervisor:
Tanner, David Ackland (Intern)
Examiner:
Fristrup, Peter (Intern)
Meldal, Morten (Ekstern)
Stockman, Robert A. (Ekstern)

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

Synthesis of novel antibacterial agents via combinatorial solid-phase synthesis

Department of Chemistry
Period: 01/11/2011 → 13/05/2015
Number of participants: 6
Phd Student:
Flagstad, Thomas (Intern)
Supervisor:
Nielsen, Thomas Eiland (Intern)
Main Supervisor:
Tanner, David Ackland (Intern)
Examiner:
Madsen, Robert (Intern)
Jensen, Knud Jørgen (Intern)
Ovaa, Huib (Ekstern)

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

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**Synthesis of Antomicrobial Natural Product Derivatives on Photlabile Solid Support**

Department of Chemistry
Period: 15/10/2011 → 26/05/2016
Number of participants: 6
Phd Student:
Mikkelsen, Remi Jacob Thomsen (Intern)
Supervisor:
Nielsen, Thomas Eiland (Intern)
Main Supervisor:
Tanner, David Ackland (Intern)
Examiner:
Duus, Jens Øllgaard (Intern)
Nielsen, John (Intern)
Ovaa, Huib (Ekstern)

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

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**Relations**
Publications:
Solid-Phase Synthesis for the Construction of Biologically Interesting Molecules and the Total Synthesis of Trioxacarcin DC-45-A2
Project: PhD

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**Green Synthesis, Characterization and Application of Metallic Nanostructures**

Department of Chemistry
Period: 01/09/2011 → 26/11/2014
Number of participants: 6
Phd Student:
Engelbrekt, Christian (Intern)
Supervisor:
Ulstrup, Jens (Intern)
Main Supervisor:
Zhang, Jingdong (Intern)
Examiner:
Harris, Pernille (Intern)
Nielsen, Michael Brorson (Intern)
Ding, Yi (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: 1/3 FUU, 1/3 inst 1/3 Andet
Project: PhD
Ruthenium-catalyzed tandem reactions
Department of Chemistry
Period: 01/09/2011 → 03/06/2015
Number of participants: 6
Phd Student:
Petersen, Mette Terp (Intern)
Supervisor:
Nielsen, Thomas Eiland (Intern)
Main Supervisor:
Tanner, David Ackland (Intern)
Examiner:
Clausen, Mads Hartvig (Intern)
Spring, David Robert (Ekstern)

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

Continuous Flow Catalysis by Supported Ionic Liquid Phase (SILP) Catalysts
Department of Chemistry
Period: 01/08/2011 → 25/03/2015
Number of participants: 6
Phd Student:
Nordvang, Emily Catherine (Intern)
Supervisor:
Riisager, Anders (Intern)
Main Supervisor:
Fehrmann, Rasmus (Intern)
Examiner:
Jensen, Anker Degn (Intern)
Pollington, Stephen D. (Ekstern)
Rasmussen, Søren Birk (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Anden EU-finansiering
Project: PhD

Simulations of Transient Dynamics
Department of Chemistry
Period: 01/08/2011 → 17/12/2014
Number of participants: 6
Phd Student:
Dohn, Asmus Ougaard (Intern)
Supervisor:
Henriksen, Niels Engholm (Intern)
Main Supervisor:
Møller, Klaus Braagaard (Intern)
Examiner:
Fristrup, Peter (Intern)
Acevedo, Olga Lucia Lopez (Ekstern)
Jensen, Jan Halborg (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: ErhvervsPhD-ordningen VTU
Project: PhD

Structural and functional characterization of protein complexes in the blood coagulation cascade

Department of Chemistry
Period: 01/08/2011 → 26/11/2014
Number of participants: 6
Phd Student:
Madsen, Jesper Jonasson (Intern)
Supervisor:
Olsen, Ole Hvilsted (Ekstern)
Main Supervisor:
Peters, Günther H.J. (Intern)
Examiner:
Kepp, Kasper Planeta (Intern)
Schiøtt, Hanne Birgti (Ekstern)
Wade, Rebecca Claire (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: ErhvervsPhD-ordningen VTU
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

New approaches to [18F] fluoride recovery and radiofluorination

Department of Chemistry
Period: 01/07/2011 → 02/09/2015
Number of participants: 6
Phd Student:
Mathiessen, Bente Ingemann (Intern)
Supervisor:
Jensen, Mikael (Intern)
Main Supervisor:
Zhuravlev, Fedor (Intern)
Examiner:
Lindvold, Lars René (Intern)
Archibald, Steve (Ekstern)
Falborg, Lise (Ekstern)

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

**Renewable Chemistry with ionic liquid-based Catalysis**
Department of Chemistry
- Period: 01/07/2011 → 30/09/2014
- Number of participants: 5
- Phd Student: Malcho, Phillip (Intern)
- Main Supervisor: Riisager, Anders (Intern)
- Examiner: Tanner, David Ackland (Intern)
- Taarning, Esben (Intern)
- Welton, Tom (Ekstern)

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

**Smart Water**
Water flooding is a standard method to extract extra oil from mature fields. International research suggests that the impact may be increased by modifying salinity or other features of the injected water. Involving industrial partners the Smart Water project led by CERE is focussed on both theoretical understanding and practical applications.

Funded by Energistyrelsen, DONG Energy and Maersk Oil

Center for Energy Resources Engineering

Department of Chemistry

Department of Civil Engineering

Section for Geotechnics and Geology
- Period: 01/06/2011 → 30/09/2014
- Number of participants: 2
- Project ID: 50845
- Project Manager, academic: Stenby, Erling Halfdan (Intern)
- Project Coordinator: Fabricius, Ida Lykke (Intern)
- Project

**Syntese af oligosakkarider relateret til plantepolysakkaridet hemicellulose**
Department of Chemistry
- Period: 01/06/2011 → 11/03/2015
- Number of participants: 5
- Phd Student: Pedersen, Martin Jæger (Intern)
- Main Supervisor: Clausen, Mads Hartvig (Intern)
- Examiner: Fristrup, Peter (Intern)
- Pedersen, Christian Marcus (Ekstern)
- Scanlan, Eoin M. (Ekstern)
Synthesis of oligo (1→5)-α-L- arabinofuranosides related to the plant polysaccharide pectin

BioRec
BioRec is a Danish research program involving several industrial and research partners. The program is focused on both Microbial Enhanced Oil Recovery (MEOR) and enzymatic enhanced oil recovery while also looking into innovative use of biotechnology in relation to prevention of corrosion and gas hydrate formation. The program is led by CERE.

Funded by HTF

NMR structural studies of oligosaccharides and other natural products
Medium Temperature Water Electrolysis

Hydrogen has the potential to provide a reliable, secure and clean source of power. Water offers a practical way of hydrogen production in association with renewable energy sources. The main challenges for water electrolysers are high cost, low efficiency and insufficient lifetime. The strategy of MEDLYS to address these issues is to develop novel materials and technologies for a medium temperature steam electrolyser operating at 200-400°C. The temperature range is optimal for 1) improving thermodynamics and kinetics of the process, 2) potentially replacing noble metal based catalysts with cost-effective alternatives, 3) allowing for a wide selection of construction materials from metals, ceramics and thermal plastics for conducting, insulating or sealing purposes and 4) maintaining long-term durability. MEDLYS will starts with development of fundamental materials including inorganic/composite proton conducting electrolyte, alternative catalysts and other construction (electrode substrate, current collector, and bipolar plate) materials. Based on the materials, electrolyser components will be manufactured and a lab-scale cell will be constructed for evaluation and concept-proof test. The proposal is based on the results from ongoing activities within DSF HyCycle Center by most of the consortium partners, who have expertise from materials science and technological know-how and strong intention to further exploit the achievements after the project. The fulfilment of MEDLYS objectives is believed to bring breakthroughs in the hydrogen production technology, which, in turn, would promote the renewable energy technologies on a national as well as an European and global level.

Department of Energy Conversion and Storage
Proton conductors
Energy and Materials
Department of Chemistry
Department of Physics
Experimental Surface and Nanomaterials Physics
University of Southern Denmark
Technical University of Munich
Danish Power Systems ApS
Tantaline A/S
Period: 01/03/2011 → 28/02/2015
Number of participants: 6
Acronym: MEDLYS
Number of related Ph.D. students: 1
Project participant:
Christensen, Erik (Intern)
Barner, Jens H. Von (Intern)
Li, Qingfeng (Intern)
Chorkendorff, Ib (Intern)
Petrushina, Irina (Intern)
Project Coordinator:
Bjerrum, Niels J. (Intern)
Project

Rational Evolution of Superstable Laccases

Department of Chemistry
Period: 01/03/2011 → 26/11/2014
Number of participants: 6
Phd Student:
Brander, Søren (Intern)
Supervisor:
Mikkelsen, Jørn Dalgaard (Intern)
Main Supervisor:
Kepp, Kasper Planeta (Intern)
Examiner:
Christensen, Hans Erik Mølager (Intern)
Bjerrum, Morten Jannik (Ekstern)
Urlacher, Vlada (Ekstern)

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

**Disc. Meeting, løbende**
Funded by: Deltagerbetaling

Center for Energy Resources Engineering

Department of Chemistry

**Period:** 01/02/2011 → 31/12/2020
- **Number of participants:** 1
- **Project ID:** 50807
- **Project Manager, academic:** Stenby, Erling Halfdan (Intern)

**Removal of Flue Gas Components with Ionic Liquids**

Master's thesis

Department of Chemistry

Centre for Catalysis and Sustainable Chemistry

**Period:** 01/02/2011 → 18/11/2011
- **Number of participants:** 1
- **Project participant:** Kolding, Helene (Intern)

**Hydrocarbon Selective Catalytic Reduction of NOx in biomass Fired Boilers**

Department of Chemistry

**Period:** 15/01/2011 → 28/05/2014
- **Number of participants:** 5
- **Phd Student:** Schill, Leonhard (Intern)
- **Main Supervisor:** Fehrmann, Rasmus (Intern)
- **Examiner:** Henriksen, Niels Engholm (Intern)
- **Boghosian, Soghomon (Ekstern)**
- **Kröcher, Oliver (Ekstern)**

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

**New Approaches to Radiofluorination using Transition Metal 18F-Fluorides**

Department of Chemistry

**Period:** 15/12/2010 → 02/07/2014
- **Number of participants:** 5
- **Phd Student:** Revunov, Evgeny V. (Intern)
- **Main Supervisor:** Zhuravlev, Fedor (Intern)
- **Examiner:** Lindvold, Lars René (Intern)
Krasikova, Raisa Nikolaevna (Ekstern)
Tanner, David Ackland (Intern)

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

Nanoscale Electrocatalysts for Chemical and Biological Sensors
Department of Chemistry
Period: 01/12/2010 → 23/04/2014
Number of participants: 6
Phd Student:
Zhu, Nan (Intern)
Supervisor:
Chi, Qijin (Intern)
Main Supervisor:
Ulstrup, Jens (Intern)
Examiner:
Horsewell, Andy (Intern)
Nielsen, Michael Brorson (Intern)
Ruzgas, Tautgirdas (Ekstern)

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

Total Synthesis and Biological Evaluation of Azumamide E and Analogs
Department of Chemistry
Period: 01/12/2010 → 03/02/2014
Number of participants: 5
Phd Student:
Villadsen, Jesper (Intern)
Main Supervisor:
Olsen, Christian Adam (Intern)
Examiner:
Tanner, David Ackland (Intern)
Ghadiri, M. Reza (Ekstern)
Strømgaard, Kristian (Ekstern)

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

Azumamide E and Analogs as Epigenetic Modulators
Department of Chemistry
Period: 01/11/2010 → 07/05/2014
Number of participants: 5
Phd Student:
Maolanon, Alex (Intern)
Main Supervisor:
Olsen, Christian Adam (Intern)
Examiner:
Nielsen, Thomas Eiland (Intern)
Poulsen, Thomas B. (Ekstern)
Organic Synthesis with Organometallic Reactions

Department of Chemistry
Period: 01/11/2010 → 28/05/2014
Number of participants: 6
Phd Student:
Christensen, Stig Holden (Intern)
Supervisor:
Holm, Torkil (Intern)
Main Supervisor:
Madsen, Robert (Intern)
Examiner:
Tanner, David Ackland (Intern)
Pittelkow, Michael (Ekstern)
Szabó, Kálman J. (Ekstern)

Design, Synthesis and Characterization of Novel Bioimetric Oligomers

Department of Chemistry
Period: 15/10/2010 → 07/05/2014
Number of participants: 5
Phd Student:
Laursen, Jonas Striegler (Intern)
Main Supervisor:
Olsen, Christian Adam (Intern)
Examiner:
Clausen, Mads Hartvig (Intern)
Albericio, Fernando (Ekstern)
Franzyk, Henrik (Intern)

Homogeneous Catalysis with Primary Alcohols

Department of Chemistry
Period: 01/10/2010 → 18/12/2013
Number of participants: 4
Phd Student:
Olsen, Esben Paul Krogh (Intern)
Main Supervisor:
Madsen, Robert (Intern)
Examiner:
Tanner, David Ackland (Intern)
Norrby, Per-Ola (Intern)

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

Department of Chemistry  
Period: 01/09/2010 → 07/05/2014  
Number of participants: 5  
PhD Student:  
Andersen, Mathias Christian Franch (Intern)  
Main Supervisor:  
Clausen, Mads Hartvig (Intern)  
Examiner:  
Madsen, Robert (Intern)  
Oscarson, Stefan (Ekstern)  
Pedersen, Christian Marcus (Ekstern)  

**Financing sources**

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

**Intermediate Temperature Proton Conducting Systems (PROCON)**

Energy and Materials  
Department of Chemistry  
Period: 01/06/2010 → 31/05/2013  
Number of participants: 6  
Acronym: PROCON  
Project participant:  
Li, Qingfeng (Intern)  
Petrushina, Irina (Intern)  
Jensen, Jens Oluf (Intern)  
Christensen, Erik (Intern)  
Cleemann, Lars Nilausen (Intern)  
Project Manager, organisational:  
Bjerrum, Niels J. (Intern)  

**Financing sources**

Source: Forsk. Andre statslige danske - Grundforskn.fonden  
Name of research programme: Forsk. Andre statslige danske - Grundforskn.fonden  
Amount: 15,000,000.00 Danish Kroner  
Project

**Computational Evolution of proteins**

Department of Chemistry  
Period: 01/05/2010 → 19/08/2013  
Number of participants: 5  
PhD Student:  
Dasmeh, Pouria (Intern)  
Main Supervisor:  
Kepp, Kasper Planeta (Intern)  
Examiner:  
Christensen, Hans Erik Mølager (Intern)  
Fago, Angela (Ekstern)  
Goldstein, Richard A. (Ekstern)  

**Financing sources**
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: Institut stipendie (DTU)
Project: PhD

Oxidative Coupling Reactions with Alcohols

Department of Chemistry
Period: 01/04/2010 → 02/07/2014
Number of participants: 5
Phd Student:
Sølvhøj, Amanda Birgitte (Intern)
Main Supervisor:
Madsen, Robert (Intern)
Examiner:
Fristrup, Peter (Intern)
Nielsen, Mogens Brøndsted (Ekstern)
Wärnmark, Kenneth (Ekstern)

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

Synthesis of Human Milk Oligosaccharides

Department of Chemistry
Period: 01/04/2010 → 23/04/2014
Number of participants: 5
Phd Student:
Jennum, Camilla Arboe (Intern)
Main Supervisor:
Madsen, Robert (Intern)
Examiner:
Gotfredsen, Charlotte Held (Intern)
Jensen, Henrik Helligsø (Ekstern)
Schmidt, Richard R. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
**Oligosaccharide synthesis**

Department of Chemistry  
Period: 15/03/2010 → 24/06/2013  
Number of participants: 6  
Phd Student: Zakharova, Alexandra (Intern)  
Supervisor: Clausen, Mads Hartvig (Intern)  
Main Supervisor: Madsen, Robert (Intern)  
Examiner: Duus, Jens Ølgaard (Intern)  
Field, Robert A. (Ekstern)  
Hindsgaul, Ole (Ekstern)

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Marie Curie (EU-stipendium)

**Rational Design of Transition Metal-based Catalysts for C-H Activation Processes**

Department of Chemistry  
Period: 15/03/2010 → 11/12/2013  
Number of participants: 4  
Phd Student: Engelin, Casper Junker (Intern)  
Main Supervisor: Fristrup, Peter (Intern)  
Examiner: Tanner, David Ackland (Intern)  
Andersson, Pher G. (Ekstern)

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

**Catalytic conversion of renewables to value-added chemicals**

Department of Chemistry  
Period: 01/03/2010 → 31/12/2011  
Number of participants: 2  
Phd Student: Eyjolfsdottir, Ester Inga (Intern)  
Main Supervisor: Riisager, Anders (Intern)

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

**Katalytisk omdannelse af biomass til flydende brændsel**

Department of Chemistry  
Period: 01/03/2010 → 19/08/2013  
Number of participants: 6
Phd Student:
Kunov-Kruse, Andreas Jonas (Intern)
Supervisor:
Riisager, Anders (Intern)
Main Supervisor:
Fehrmann, Rasmus (Intern)
Examiner:
Møller, Klaus Braagaard (Intern)
Beato, Pablo (Ekstern)
Rogers, Robin D. (Ekstern)

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

To explore large-scale and low-cost nano-processing technology and eventually to prepare a broad range of orderly nano-size functional structures

Department of Chemistry

NanoChemistry
Period: 01/02/2010 → 31/01/2011
Number of participants: 2
Project participant:
Hao, Xian (Intern)
Project Coordinator:
Zhang, Jingdong (Intern)

Green Synthesis, Characterization and Application of Metallic Nanostructures

Department of Chemistry

NanoChemistry
Period: 01/01/2010 → 31/12/2012
Number of participants: 3
Project participant:
Engelbrekt, Christian (Intern)
Jensen, Palle Skovhus (Intern)
Project Coordinator:
Zhang, Jingdong (Intern)

Bioorganic Chemistry

Department of Chemistry
Period: 01/01/2010 → 19/08/2013
Number of participants: 5
Phd Student:
Viart, Helene Marie-France (Intern)
Main Supervisor:
Clausen, Mads Hartvig (Intern)
Examiner:
Tanner, David Ackland (Intern)
Nielsen, Poul (Ekstern)
Wärnmark, Kenneth (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Institut stipendie (DTU)
Project: PhD
CERE Administration
Center for Energy Resources Engineering
Department of Chemistry
Period: 01/01/2010 → 10/10/2020
Number of participants: 1
Project ID: 50678
Project participant:
Stenby, Erling Halfdan (Intern)

Conical Intersections and Excited State Dynamics
Department of Chemistry
Period: 01/01/2010 → 19/04/2013
Number of participants: 6
Phd Student:
Kuhlman, Thomas Scheby (Intern)
Supervisor:
Sølling, Theis Ivan (Intern)
Main Supervisor:
Møller, Klaus Braagaard (Intern)
Examiner:
Henriksen, Niels Engholm (Intern)
Christiansen, Ove (Ekstern)
Weber, Peter M. (Ekstern)

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

Organic Synthesis of antimicrobial agents and antibiotics
Department of Chemistry
Period: 01/01/2010 → 19/08/2013
Number of participants: 5
Phd Student:
Hansen, Mette Reimert (Intern)
Main Supervisor:
Nielsen, Thomas Eiland (Intern)
Examiner:
Olsen, Christian Adam (Intern)
Nielsen, John (Intern)
Stockman, Robert A. (Ekstern)

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

Direct Synthesis of Amides from Alcohols and Amines
Department of Chemistry
Period: 01/12/2009 → 24/06/2013
Number of participants: 6
Phd Student:
Makarov, Ilya (Intern)
Supervisor:
Fristrup, Peter (Intern)
Main Supervisor:
Madsen, Robert (Intern)
Examiner:
Tanner, David Ackland (Intern)
Jørgensen, Karl Anker (Ekstern)
Wendt, Ola F. (Ekstern)

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

Chemical specification of the long-lived radionuclide technetium-99 and its environment behaviour

Department of Chemistry
Period: 01/11/2009 → 17/12/2012
Number of participants: 7
Phd Student:
Shi, Keliang (Intern)

Supervisor:
Roos, Per (Intern)
Wu, Wangsou (Ekstern)
Main Supervisor:
Hou, Xiaolin (Intern)
Examiner:
Egsgaard, Helge (Intern)
Croudace, Ian W. (Ekstern)
Goutelard, Florence (Ekstern)

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

Dehydrogenative Coupling of Alcohols and Amines

Department of Chemistry
Period: 01/11/2009 → 19/03/2013
Number of participants: 5
Phd Student:
Maggi, Agnese (Intern)

Main Supervisor:
Madsen, Robert (Intern)
Examiner:
Clausen, Mads Hartvig (Intern)
Jensen, Henrik Helligsø (Ekstern)
Somfai, Peter (Ekstern)

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

Sustainable catalysis with functional ionic liquids

Department of Chemistry
Period: 01/11/2009 → 24/06/2013
Number of participants: 5
Phd Student:
Integrated Chemical Synthesis and Cell Screening in Patient Cells

Department of Chemistry
Period: 15/10/2009 → 31/03/2014
Number of participants: 2
Phd Student:
Taveras, Kennedy (Intern)
Main Supervisor:
Nielsen, Thomas Eiland (Intern)

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

Atomistic Modelling of Chemical Reactions - A New Approach in Drug Design

Department of Chemistry
Period: 01/10/2009 → 30/09/2013
Number of participants: 5
Phd Student:
Corozzi, Alessandro (Intern)
Main Supervisor:
Fristrup, Peter (Intern)
Examiner:
Henriksen, Niels Engholm (Intern)
Ahlquist, Märten Sten Gösta (Intern)
Jensen, Jan Halborg (Ekstern)

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

Catalytic routes to renewable plasticizers

Department of Chemistry
Period: 01/10/2009 → 13/11/2014
Number of participants: 2
Phd Student:
Sørensen, Mathilde Grau (Intern)
Main Supervisor:
Riisager, Anders (Intern)

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

Plasticisers are additives that increase the plasticity of the materials to which they are added. Plasticisers are widely used in the plastic industry to plasticise polymers like PVC and PLA. Phthalates, based on non sustainable petrochemical raw materials are the most widely used group of plasticisers. However, phthalates have low biodegradability and negative effects on the environment, where hormonal disrupting effects on higher animals such as fish, mammals and humans is the most alarming, causing abnormalities in the reproductive system. It is therefore desirable to be able to produce alternative sustainable plasticisers the price of which, should be at competitive levels to that of phthalates. The role of Department of Toxicology and Risk Assessment in the project is evaluation of toxic properties of potential compounds generated in the project using based on structure-toxicity relationship in silico ((Q)SAR), testing of the potential genotoxicity of synthesized compound(s) in vitro, and of the potential anti-androgenic effects in vivo in prenatally exposed rats.

Department of Chemistry
Division of Toxicology and Risk Assessment
National Food Institute
Aarhus University

Danisco AS
Period: 01/09/2009 → 31/08/2012
Number of participants: 1
Project participant:
Mortensen, Alicja (Intern)

**DeNOx katalysatorer til biomassefyring**

Department of Chemistry
Period: 01/08/2009 → 21/05/2013
Number of participants: 7
Phd Student:
Kristensen, Steffen Buus (Intern)
Supervisor:
Jensen, Jørgen Nørklit (Ekstern)
Riisager, Anders (Intern)
Main Supervisor:
Fehrmann, Rasmus (Intern)
Examiner:
Jensen, Anker Degn (Intern)
Bañares, Miguel A. (Ekstern)
Odenbrand, Ingemar (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: ErhvervsPhD-ordningen VTU
Project: PhD

**Diversity-Oriented Synthesis of Small Molecules Trageting Bacterial Biofilm**

Department of Chemistry
Period: 01/08/2009 → 17/12/2012
Number of participants: 4
Phd Student:
Komnatnyy, Vitaly V. (Intern)
Main Supervisor:
Nielsen, Thomas Eiland (Intern)
Examiner:
Tanner, David Ackland (Intern)
Spring, David Robert (Ekstern)
Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Diversity-Oriented Synthesis of Composite Antimicrobial Agents
Department of Chemistry
Period: 01/05/2009 → 17/08/2012
Number of participants: 5
Phd Student:
Ascic, Erhad (Intern)
Main Supervisor:
Nielsen, Thomas Eiland (Intern)
Examiner:
Madsen, Robert (Intern)
Nelson, Adam S. (Ekstern)
Skrydstrup, Troels (Ekstern)

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

Danish high temperature PEMFC components, MEA and stack
Energy and Materials
Department of Chemistry
Energinet.dk
Danish Power Systems ApS
IRD Fuel Cells A/S
Dantherm Power A/S
Period: 01/04/2009 → 31/03/2013
Number of participants: 9
Acronym: HotMEA
Project ID: 40469
Project participant:
Li, Qingfeng (Intern)
Jensen, Jens Oluf (Intern)
Permyakova, Anastasia Aleksandrovna (Intern)
Behnke, Kim (Ekstern)
Steenberg, Thomas (Ekstern)
Lundgaard, Jørgen (Ekstern)
Thomsen, Jesper (Ekstern)
Albæk, Per (Ekstern)
Project Manager, organisational:
Bjerrum, Niels J. (Intern)

Financing sources
Source: Forskningsprojekter - Miljø- og Energiministeriet
Name of research programme: Forskningsprojekter - Miljø- og Energiministeriet
Project

Design, Synthesis and Biological Evaluation of Histone Demethylase Inhibitors
Department of Chemistry
Period: 01/03/2009 → 20/08/2012
Number of participants: 5
Phd Student:
Cohrt, Anders Emil O'Hanlon (Intern)
Main Supervisor:
Nielsen, Thomas Eiland (Intern)
Examiner:
Olsen, Christian Adam (Intern)
Benito, Juan M. (Ekstern)
Nielsen, John (Intern)

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

Electronic Properties of DNA-based Molecules - Single-molecule nanoscience
Department of Chemistry
Period: 01/03/2009 → 17/12/2012
Number of participants: 6
Phd Student:
Salvatore, Princia (Intern)
Supervisor:
Hansen, Allan Glargaard (Intern)
Main Supervisor:
Ulstrup, Jens (Intern)
Examiner:
Kneipp, Katrin (Intern)
Friis, Esben P. (Intern)
Wollenberger, Ulla (Ekstern)

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

Ionic Liquids for CO2 Capture
Funded by FIST, DONG Energy and Mærsk Oil
DOC 09/00224

Under lukning
Center for Energy Resources Engineering
Department of Chemistry
Period: 01/03/2009 → 01/06/2011
Number of participants: 1
Acronym: Ionic Liquids
Project ID: 50644
Project participant:
Stenby, Erling Halfdan (Intern)

Kemisk Dynamik: Observation og kontrol
Department of Chemistry
Period: 01/03/2009 → 30/09/2012
Number of participants: 6
Phd Student:
Petersen, Jakob (Intern)
Supervisor:
Henriksen, Niels Engholm (Intern)
Main Supervisor:
Møller, Klaus Braagaard (Intern)
Examiner:
Peters, Günther H.J. (Intern)
Engel, Volker (Ekstern)
Jørgensen, Solvejg (Ekstern)

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

Combining X-ray diffraction and absorption for studies of metalloproteins
Department of Chemistry
Period: 01/01/2009 → 24/05/2012
Number of participants: 6
Phd Student:
Frankær, Christian Grundahl (Intern)
Supervisor:
Harris, Pernille (Intern)
Main Supervisor:
Ståhl, Kenny (Intern)
Examiner:
Peters, Günther H.J. (Intern)
Ascone, Isabella (Ekstern)
Birkedal, Henrik (Ekstern)

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

Methanol Carbonylation by SILP Catalysis
Department of Chemistry
Period: 01/12/2008 → 19/09/2012
Number of participants: 6
Phd Student:
Hanning, Christopher William (Intern)
Supervisor:
Riisager, Anders (Intern)
Main Supervisor:
Fehrmann, Rasmus (Intern)
Examiner:
Berg, Rolf W. (Intern)
Boghosian, Soghomon (Ekstern)
Vogel, Stefan (Ekstern)

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

UV-Raman Spectroscopy of Crude oil Mixtures, biological samples and catalysts, a fibre optical method for materials characterization
Department of Chemistry
Period: 15/11/2008 → 14/03/2012
Number of participants: 5
Phd Student:
Liu, Chuan (Intern)
Main Supervisor:
Berg, Rolf W. (Intern)
Examiner:
Andersen, Jens (Intern)
Hassing, Søren (Ekstern)
Kiefer, Johannes (Ekstern)

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

CompSim
DOC 08/00420
prolonged until 30. april 2012
Center for Energy Resources Engineering
Department of Chemistry
Period: 10/11/2008 → 09/11/2010
Number of participants: 1
Project ID: 50588
Project participant:
Stenby, Erling Halfdan (Intern)

Udtrykkelse, oprensning og karakterisering af metalloenzymer involveret i neurophsykiatriske sygdomme
Department of Chemistry
Period: 15/10/2008 → 19/09/2012
Number of participants: 4
Phd Student:
Haahr, Lærke Tvedebrink (Intern)
Main Supervisor:
Christensen, Hans Erik Mølager (Intern)
Examiner:
Ulstrup, Jens (Intern)
Thunnissen, Marjolein (Ekstern)

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

Development of New Methods for the Synthesis of Biologically Active small Molecules
Department of Chemistry
Period: 01/10/2008 → 18/04/2012
Number of participants: 5
Phd Student:
Petersen, Rico (Intern)
Main Supervisor:
Nielsen, Thomas Eiland (Intern)
Examiner:
Tanner, David Ackland (Intern)
Jensen, Knud Jørgen (Intern)
Looper, Ryan E. (Ekstern)

Financing sources
Source: Internal funding (public)
New Polymeric Electrolytes for application in water electrolysis

Department of Chemistry
Period: 15/08/2008 → 28/09/2011
Number of participants: 8
Phd Student:
Aili, David (Intern)
Supervisor:
Barner, Jens H. Von (Intern)
Christensen, Erik (Intern)
Li, Qingfeng (Intern)
Main Supervisor:
Bjerrum, Niels J. (Intern)
Examiner:
Berg, Rolf W. (Intern)
Bleha, Miroslav (Ekstern)
Steenberg, Thomas (Intern)

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

Single-Molecule Enzyme Dynamics and New Biosensing Devices

Department of Chemistry
Period: 01/07/2008 → 08/02/2012
Number of participants: 6
Phd Student:
Ikemoto, Hideki (Intern)
Supervisor:
Chi, Qijin (Intern)
Main Supervisor:
Ulstrup, Jens (Intern)
Examiner:
Fehrmann, Rasmus (Intern)
Nielsen, Michael Brorson (Intern)
Ivaska, Ari Usko (Ekstern)

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

Chemicals from Renewables

Department of Chemistry
Period: 15/06/2008 → 21/09/2011
Number of participants: 5
Phd Student:
Ståhlberg, Tim Johannes Bjarki (Intern)
Main Supervisor:
Rüsager, Anders (Intern)
Examiner:
Tanner, David Ackland (Intern)
Rogers, Robin D. (Ekstern)
Taarning, Esben (Intern)
New Electrocatalytic Materials in water electrolysis/Udvikling og test af nye elektrodematerialer til vandelektrolyse

Department of Chemistry
Period: 15/06/2008 → 21/09/2011
Number of participants: 7
Phd Student:
Nikiforov, Aleksey Valerievich (Intern)
Supervisor:
Christensen, Erik (Intern)
Petrushina, Irina (Intern)
Main Supervisor:
Bjerrum, Niels J. (Intern)
Examiner:
Barner, Jens H. Von (Intern)
Bouzek, Karel (Ekstern)
Skou, Eivind Morten (Ekstern)

Catalytic Routes to Renewable Polymer Building Blocks

Department of Chemistry
Period: 01/06/2008 → 14/12/2011
Number of participants: 6
Phd Student:
Hansen, Thomas Søndergaard (Intern)
Supervisor:
Woodley, John (Intern)
Main Supervisor:
Røsager, Anders (Intern)
Examiner:
Clausen, Mads Hartvig (Intern)
Bols, Mikael (Ekstern)
Leitner, Walter (Ekstern)

Ligand Binding and Activation Mechanism of the Glucagon-Like Peptide-1 Receptor

Department of Chemistry
Period: 01/06/2008 → 21/05/2013
Number of participants: 6
Phd Student:
Underwood, Christina Rye (Intern)
Supervisor:
Reedtz-Runge, Steffen (Ekstern)
Main Supervisor:
Peters, Günther H.J. (Intern)
Examiner:
Christensen, Hans Erik Mølager (Intern)
Donnelly, Daniel (Ekstern)
Gether, Ulrik (Ekstern)

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

Bio-Petrochemicals
Department of Chemistry
Period: 01/04/2008 → 08/02/2012
Number of participants: 6
Phd Student:
Gorbanev, Yury (Intern)
Supervisor:
Woodley, John (Intern)
Main Supervisor:
Riisager, Anders (Intern)
Examiner:
Fristrup, Peter (Intern)
Grunwaldt, Jan-Dierk (Intern)
Herbst, Konrad (Ekstern)

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

Organometallic Reactions in Organic Synthesis
Department of Chemistry
Period: 01/04/2008 → 08/02/2012
Number of participants: 6
Phd Student:
Osztrovszky, Gyorgyi (Intern)
Supervisor:
Holm, Torkil (Intern)
Main Supervisor:
Madsen, Robert (Intern)
Examiner:
Tanner, David Ackland (Intern)
Jensen, Henrik Helligsø (Ekstern)
Thiem, Joachim Erich (Ekstern)

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

Udtrykkelse, oprensning og karakterisering af metal-holdige Monooxygenaser involveret i neuropsykiatriske sygdommer
Department of Chemistry
Period: 01/04/2008 → 30/09/2013
Number of participants: 5
Phd Student:
Vendelboe, Trine Vammen (Intern)
Main Supervisor:
Christensen, Hans Erik Mølager (Intern)
Examiner:
Peters, Günther H.J. (Intern)
Amzel, L. Mario (Ekstern)
Kastrup, Jette Sandholm J. (Ekstern)

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

**Biological Surfaces and Bacterial Biofilms Investigated by Atomic Force Microscopy**

Department of Chemistry  
**Period:** 01/03/2008 → 27/06/2012  
**Number of participants:** 6  
**Phd Student:**  
Hu, Yifan (Intern)  
**Supervisor:**  
Zhang, Jingdong (Intern)  
**Main Supervisor:**  
Ulstrup, Jens (Intern)  
**Examiner:**  
Christensen, Hans Erik Mølager (Intern)  
Arnebrant, Thomas (Ekstern)  
Mortensen, John (Ekstern)

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

**Extending the Functional Diversity of Iron-Sulfur Proteins by Generation of Heterometallic-Iron-Sulfur Clusters**

Department of Chemistry  
**Period:** 01/02/2008 → 11/05/2011  
**Number of participants:** 6  
**Phd Student:**  
Martic, Maja (Intern)  
**Supervisor:**  
Ooi, Bee Lean (Intern)  
**Main Supervisor:**  
Christensen, Hans Erik Mølager (Intern)  
**Examiner:**  
Ulstrup, Jens (Intern)  
Bjerrum, Morten Jannik (Ekstern)  
Gyurcsik, Béla (Ekstern)

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

**Speciation and Environmental Behaviour of Radionuclides**

Department of Chemistry  
**Period:** 01/02/2008 → 08/02/2012  
**Number of participants:** 5  
**Phd Student:**  
Hansen, Violeta (Intern)  
**Main Supervisor:**  
Roos, Per (Intern)  
**Examiner:**  
Nielsen, Sven Poul (Intern)
Holm, G. Elis G. (Ekstern)
Sturup, Stefan (Intern)

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

Study of new inexpensive materials for robust oxygen sensor electrodes

Department of Chemistry
Period: 01/02/2008 → 24/08/2011
Number of participants: 7
PhD Student:
Lund, Anders (Intern)
Supervisor:
Hansen, Karin Vels (Intern)
Mogensen, Mogens Bjerg (Intern)
Main Supervisor:
Skaarup, Steen (Intern)
Examiner:
Holtappels, Peter (Intern)
Skou, Eivind Morten (Ekstern)
Wiemhöfer, Hans-Dieter (Ekstern)

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

Ultra Porous Zeolites: Structure-Activity Relations

Department of Chemistry
Period: 01/02/2008 → 15/06/2011
Number of participants: 8
PhD Student:
Holm, Martin Spangsberg (Intern)
Supervisor:
Bjørgen, Morten (Ekstern)
Christensen, Claus H. (Intern)
Kustova, Marina (Intern)
Main Supervisor:
Fehrmann, Rasmus (Intern)
Examiner:
Ståhl, Kenny (Intern)
Glasius, Marianne (Ekstern)
Pérez-Ramírez, Javier (Ekstern)

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

Catalytic Production of Biodiesel

Department of Chemistry
Period: 01/01/2008 → 30/09/2011
Number of participants: 5
PhD Student:
Madsen, Anders Theilgaard (Intern)
Rationelt design af metalloproteiner af katalytisk relevans - strukturelle og funktionelle studier af molybdænaloger af jern-svovl proteiner

Department of Chemistry
Number of participants: 7
PhD Student:
Løvgreen, Monika Nøhr (Intern)
Supervisor:
Ooi, Bee Lean (Intern)
Christensen, Hans Erik Mølager (Intern)
Main Supervisor:
Harris, Pernille (Intern)
Examiner:
Martinussen, Jan (Intern)
Bergfors, Terese (Ekstern)
Johansson, Eva (Ekstern)

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

ADORE - Advanced Oil Recovery Methods
As easily accessible oil reserves are becoming scarcer, the need for new approaches in Enhanced Oil Recovery (EOR) is growing. The Advanced Oil Recovery Methods (ADORE) project led by CERE encompasses a range of research disciplines with the objective of adding to recoverable hydrocarbon reserves via novel or improved EOR methodologies.

Funded by FIST
Center for Energy Resources Engineering

Department of Chemistry
Period: 01/09/2007 → 01/01/2013
Number of participants: 1
Acronym: ADORE
Project ID: 50548
Project Manager, academic:
Stenby, Erling Halfdan (Intern)
Project

X-ray investigation of pharmaceuticals

Department of Chemistry

Egalet A/S
Period: 27/08/2007 → 31/12/2008
Number of participants: 2
Contact person:
Lyhne-Iversen, Louise (Ekstern)
Project Manager, organisational:
Ståhl, Kenny (Intern)

Financing sources
Source: Indtægtsdækket virksomhed UK 90
Name of research programme: Indtægtsdækket virksomhed UK 90
Amount: 50,000.00 Danish Kroner

Mesoporous Molecular Sieve Catalysts
Department of Chemistry
Number of participants: 6
PhD Student:
Højholt, Karen Thrane (Intern)
Supervisor:
Nielsen, Michael Brorson (Intern)
Main Supervisor:
Fehrmann, Rasmus (Intern)
Examiner:
Ståhl, Kenny (Intern)
Pérez-Ramírez, Javier (Ekstern)
Vogel, Stefan (Ekstern)

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

Theory and Modelling of Ultrafast x-ray Imaging of Dynamical Non-Equilibrium Systems
Department of Chemistry
Period: 01/08/2007 → 24/11/2010
Number of participants: 6
PhD Student:
Lorenz, Ulf (Intern)
Supervisor:
Møller, Klaus Braagaard (Intern)
Main Supervisor:
Henriksen, Niels Engholm (Intern)
Examiner:
Hansen, Flemming Yssing (Intern)
Engel, Volker (Ekstern)
Tschentscher, Thomas (Ekstern)

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

Bio-Petrochemicals
Department of Chemistry
Period: 01/07/2007 → 29/02/2008
Number of participants: 2
PhD Student:
Marsden, Charlotte Clare (Intern)
Main Supervisor:
Christensen, Claus H. (Intern)
Financing sources
Source: Internal funding (public)
Name of research programme: DTU, Samfinansiering
Project: PhD

Metalloproteiner involveret i neurologiske sygdomme - karakterisering af det jernholdige enzym tryphanhydroxylase

Department of Chemistry
Period: 01/07/2007 → 30/09/2010
Number of participants: 5
Phd Student:
Boesen, Jane (Intern)
Main Supervisor:
Christensen, Hans Erik Mølager (Intern)
Examiner:
Peters, Günther H.J. (Intern)
Caspersen, Mikael Bjerg (Intern)
Sobott, Frank (Ekstern)

Synthesis of Heterocycles from Alcohols and Amines

Department of Chemistry
Period: 01/07/2007 → 30/09/2009
Number of participants: 3
Phd Student:
Tursky, Matyas (Intern)
Supervisor:
Christensen, Claus H. (Intern)
Main Supervisor:
Madsen, Robert (Intern)

X-ray investigations of pharamaceuticals

Department of Chemistry
GEA Pharmaceuticals A/S
Period: 01/07/2007 → 31/12/2010
Number of participants: 2
Project ID: 40229
Contact person:
Fischer, Erik (Ekstern)
Project Manager, organisational:
Ståhl, Kenny (Intern)

Financing sources
Source: Indtægtsdækket virksomhed UK 90
Name of research programme: Indtægtsdækket virksomhed UK 90
Amount: 94,750.00 Danish Kroner
Project

Alternative Alkali Resistant deNox Technologies
Department of Chemistry
Period: 01/06/2007 → 01/09/2010
Number of participants: 6
Phd Student:
Due-Hansen, Johannes (Intern)
Supervisor:
Riisager, Anders (Intern)
Main Supervisor:
Fehrmann, Rasmus (Intern)
Examiner:
Henriksen, Niels Engholm (Intern)
Kröcher, Oliver (Ekstern)
Jensen, Joakim Reimer (Intern)

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

Production of Hydrogen by Electrolysis
Department of Chemistry
Period: 01/06/2007 → 15/10/2008
Number of participants: 4
Phd Student:
Wonsyld, Karen (Intern)
Supervisor:
Jensen, Jens Oluf (Intern)
Petrushina, Irina (Intern)
Main Supervisor:
Bjerrum, Niels J. (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: 1/3 DTU-stip, 2/3 FUR/andet
Project: PhD

Control of Hordein Breakdown in Brewing
Department of Chemistry
Period: 01/05/2007 → 13/04/2011
Number of participants: 6
Phd Student:
Munch, Astrid (Intern)
Supervisor:
Olsen, Ole (Ekstern)
Main Supervisor:
Christensen, Hans Erik Mølager (Intern)
Examiner:
Finnie, Christine (Intern)
Krupinska, Karin (Ekstern)
Poulsen, Charlotte H. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: ErhvervsPhD-ordningen VTU
Project: PhD

Tools for Chemical Biology: New Macrocyclic Antibiotics from Diversity Oriented Synthesis
Department of Chemistry  
Period: 01/04/2007 → 24/11/2010  
Number of participants: 6  
PhD Student:  
Madsen, Charlotte Marie (Intern)  
Supervisor:  
Gotfredsen, Charlotte Held (Intern)  
Main Supervisor:  
Clausen, Mads Hartvig (Intern)  
Examiner:  
Nielsen, Thomas Eiland (Intern)  
Nelson, Adam S. (Ekstern)  
Nielsen, John (Intern)  

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

Liposomale prodrugsystemer - syntese, biofysiske og biologiske studier  
Department of Chemistry  
Period: 01/03/2007 → 01/09/2010  
Number of participants: 7  
PhD Student:  
Pedersen, Palle Jacob (Intern)  
Supervisor:  
Andresen, Thomas Lars (Intern)  
Madsen, Robert (Intern)  
Main Supervisor:  
Clausen, Mads Hartvig (Intern)  
Examiner:  
Tanner, David Ackland (Intern)  
Jensen, Knud Jørgen (Intern)  
Thompson, David H. (Ekstern)  

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

Investigation of the Influence of Group II Elements on Human Health - New Analytical Methods for Development of Strontium Pharmaceuticals  
Department of Chemistry  
Period: 01/02/2007 → 08/06/2011  
Number of participants: 5  
PhD Student:  
Raffalt, Anders Christer (Intern)  
Main Supervisor:  
Andersen, Jens (Intern)  
Examiner:  
Henriksen, Niels Engholm (Intern)  
Leito, Ivo (Ekstern)  
Marie, Pierre J. (Ekstern)  

Financing sources  
Source: Internal funding (public)  
Name of research programme: DTU-lønnet stipendie  
Project: PhD
Towards & Methanol Economy
Department of Chemistry
Period: 01/02/2007 → 09/02/2011
Number of participants: 5
Phd Student:
Mentzel, Uffe Vie (Intern)
Main Supervisor:
Fehrmann, Rasmus (Intern)
Examiner:
Ståhl, Kenny (Intern)
Beato, Pablo (Ekstern)
Bjørgen, Morten (Ekstern)

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

Metalorganiske reaktioner med alkoholer
Department of Chemistry
Period: 01/01/2007 → 23/05/2012
Number of participants: 5
Phd Student:
Lorentz-Petersen, Linda Luise Reeh (Intern)
Main Supervisor:
Madsen, Robert (Intern)
Examiner:
Olsen, Christian Adam (Intern)
Andersson, Pher G. (Ekstern)
Kristensen, Jesper Langgaard (Ekstern)

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

Øget olieudvinding gennem CO2 udnyttelse
Center for Energy Resources Engineering
Department of Chemistry
Period: 01/01/2007 → 31/12/2009
Number of participants: 1
Project ID: 50505
Project Manager, academic:
Stenby, Erling Halfdan (Intern)
Project

Rationelt design af metalloproteiner af katalytisk relevans - syntese og karakterisering af molybdænanalager af jern-svovl proteiner
Department of Chemistry
Period: 01/01/2007 → 01/09/2010
Number of participants: 8
Phd Student:
Kristensen, Jytte (Intern)
Supervisor:
Ooi, Bee Lean (Intern)
Syntetiske GLP-1 analoger

Department of Chemistry
Period: 01/01/2007 → 21/04/2010
Number of participants: 6
PhD Student:
Storgaard, Morten (Intern)
Supervisor:
Peschke, Bernd (Ekstern)
Main Supervisor:
Tanner, David Ackland (Intern)
Examiner:
Nielsen, Thomas Eiland (Intern)
Greve, Daniel R. (Intern)
Rademann, Jörg (Ekstern)

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

X-ray investigation of pharmaceuticals

Department of Chemistry
Niels Clauson-Kaas A/S
Period: 22/12/2006 → 31/12/2008
Number of participants: 2
Contact person:
Alster, Karol (Ekstern)
Project Manager, organisational:
Ståhl, Kenny (Intern)

Financing sources
Source: Indtægtsdækket virksomhed UK 90
Name of research programme: Indtægtsdækket virksomhed UK 90
Amount: 50,000.00 Danish Kroner
Project

New Technologies for Water Electrolysis
"Midler til forberedelse af ansøgninger til EU-forskningsmidler"

Department of Chemistry
Period: 01/12/2006 → 30/06/2007
Number of participants: 1
Project ID: 40359
Project Manager, organisational:
Bjerrum, Niels J. (Intern)
Investigation of Ph(o) Complexes in Homogeneous Catalysis

Department of Chemistry
Period: 01/10/2006 → 10/02/2010
Number of participants: 7
PhD Student:
Henriksen, Signe Teuber (Intern)
Supervisor:
Fristrup, Peter (Intern)
Norrby, Per-Ola (Intern)
Main Supervisor:
Tanner, David Ackland (Intern)
Examiner:
Madsen, Robert (Intern)
Olsen, Lars (Intern)
Szabó, Kálmán J. (Ekstern)

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

Syntese og biologiske studier af lipid-baserede lægemidler

Department of Chemistry
Period: 01/10/2006 → 30/06/2007
Number of participants: 4
PhD Student:
Jørgensen, Pernille Nyvang (Intern)
Supervisor:
Andresen, Thomas Lars (Intern)
Peters, Günther H.J. (Intern)
Main Supervisor:
Madsen, Robert (Intern)

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

Sponsorer til IVC-SEP

Center for Energy Resources Engineering
Department of Chemistry
Period: 01/09/2006 → 10/10/2020
Number of participants: 1
Project ID: 50767
Project Manager, academic:
Stenby, Erling Halfdan (Intern)

Spektrokopisk karakterisering af det evolutionært oprindelige jern-svovl protein - det ældst kendte protein og dettes relation til livets oprindelse
Synthesis and Applications of Bioconjugated Metal Nanoparticles for Nanoscale Bioelectronics

Department of Chemistry
Period: 01/07/2006 → 09/02/2011
Number of participants: 6
Phd Student:
Jensen, Palle Skovhus (Intern)
Supervisor:
Chi, Qijin (Intern)
Main Supervisor:
Ulstrup, Jens (Intern)
Examiner:
Fehrmann, Rasmus (Intern)
Gorton, Lo Gunnar Otto (Ekstern)
Mølhave, Kristian (Intern)

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

Hydrogen from Metal Ammines

Department of Chemistry
Period: 01/06/2006 → 23/09/2009
Number of participants: 6
Phd Student:
Klerke, Asbjørn (Intern)
Supervisor:
Christensen, Claus H. (Intern)
Main Supervisor:
Fehrmann, Rasmus (Intern)
Examiner:
Jacobsen, Torben (Ekstern)
Nielsen, Michael Brorson (Intern)
Wasserscheid, Peter (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Grundforskningsfonden
Project: PhD
Modelling of CO2 Capture
Funded by FIST, DONG Energy and Maersk Oil

Under lukning

Center for Energy Resources Engineering

Department of Chemistry
Period: 01/05/2006 → 01/07/2010
Number of participants: 1
Project ID: 50421
Project Manager, academic:
Stenby, Erling Halfdan (Intern)

Metalorganiske Aminieringsreaktioner

Department of Chemistry
Period: 01/04/2006 → 22/10/2009
Number of participants: 5
Phd Student:
Jensen, Thomas (Intern)
Main Supervisor:
Madsen, Robert (Intern)
Examiner:
Clausen, Mads Hartvig (Intern)
Skrydstrup, Troels (Ekstern)
Wärnmark, Kenneth (Ekstern)

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

Modeling of Neurotransmitter Transporters

Department of Chemistry
Period: 01/04/2006 → 30/06/2009
Number of participants: 4
Phd Student:
Jørgensen, Anne Marie (Intern)
Supervisor:
25_NN_Studenter/Øvrige medarb. (Ekstern)
Tagmose, Lena (Ekstern)
Main Supervisor:
Peters, Günther H.J. (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: ErhvervsPhD-ordningen VTU
Project: PhD

Metalorganiske Allyleringsreaktioner

Department of Chemistry
Period: 01/03/2006 → 23/09/2009
Number of participants: 5
Phd Student:
Dam, Johan Hygum (Intern)
Main Supervisor:
Madsen, Robert (Intern)
Examiner:
Tanner, David Ackland (Intern)
Moberg, Christina (Ekstern)
Norrby, Per-Ola (Intern)

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

Metal-containing Mono-oxygenases Involved in Neurological disorders - expression in Eukaryotic Systems, purification and characterization
Department of Chemistry
Period: 01/02/2006 → 20/10/2010
Number of participants: 5
Phd Student:
Karlsen, Pernille Efferbach (Intern)
Main Supervisor:
Christensen, Hans Erik Mølager (Intern)
Examiner:
Jacobsen, Susanne (Intern)
Gajhede, Michael (Ekstern)
Raven, Emma (Ekstern)

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

Tools for Chemical Biology: New Macrocyclic Antibiotics from Diversity Oriented Synthesis
Department of Chemistry
Period: 01/02/2006 → 31/12/2006
Number of participants: 3
Phd Student:
Boet efter, John Magnus (Ekstern)
Supervisor:
Clausen, Mads Hartvig (Intern)
Main Supervisor:
Gotfredsen, Charlotte Held (Intern)

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

Dry, Intrinsic proton conducting membranes for fuel cells
Department of Chemistry
University of Copenhagen
Danish Polymer Center
Danish Power Systems ApS
Period: 01/01/2006 → 31/12/2008
Number of participants: 6
Project participant:
Li, Qingfeng (Intern)
Jensen, Jens Oluf (Intern)
Begstrup, Michael (Ekstern)
Planckett, David Victor (Ekstern)
Steenberg, Thomas (Ekstern)
Project Manager, organisational:
Bjerrum, Niels J. (Intern)

Financing sources
Source: Forskningsrådene - STVF
Name of research programme: Forskningsrådene - STVF
Amount: 1,258,131.00 Danish Kroner
Project

Raman spectroscopy by use of UltraViolet Radiation : A new useful way to avoid fluorescence
Fluorescence has been a persistent problem in Raman spectroscopy. To avoid the problems a way to seems to have opened now: Excitation with deeply ultraviolet light. "Fluorescence does not appear to exist if the exciting light has a wavelength shorter than 260 nm" [cit. S. A. Asher]. Affordable pulsed deep-UV lasers have recently been introduced to the market by a company "Photon Systems" in California. So-called HeAg og NeCu hollow-cathode lasers during operation create a metal vapor mixed with an inactive rare gas by a process reminding of sputtering. The lasers emit quasi-continuous laser light in the deep UV-range, with wavelengths of 224 nm (for silver) and 248 nm (for copper). During operation they require little electrical power and no water cooling. New instrument needed. We apply for a dedicated UV Raman-spectrometer with quartz optics, UV grating and detectors, and the necessary helping utensils. One important new aspect of the method is to introduce optical fibers, so that the optics can be totally encapsulated to avoid any deep UV radiation damage to objects and persons in the neighbourhood. UV-Raman spectroscopy will have many future applications. We will try the technique in three limited, well-defined research fields with a high content of new and innovative ideas. Hence, we want a new laser to abate fluorescence. We would like to use the new system in this way: 1) Characterisation of new waveguides by use of hollow microstructured crystal fibers. It ranges from analysis of Ge-nano-clusters embedded in silica-on-silicon planar waveguides to chemical and biological molecular identification. Samples will be prepared and investigated to find better methods to prepare silica materials with enhanced third order nonlinearity. Size and distribution of the nano-clusters are important parameters. In contrast to other methods, UV-Raman spectroscopy needs no specimen preparation and should be a non-destructive, efficient method to find the size distribution of even very small nano-clusters. The UV Raman will be tried using hollow micro-structured optical fibers. Such air-hole fibers should enable easy and safe UV spectroscopy. This entirely new concept will be tried as well as fibers designed such that the air holes are used both for light guiding and at the same time as pipettes for a chemical solution (like gasoline/methanol mixes) that one wants to analyse (co-work with COM-center). 2) Characterisation of fluorescing crude oil mixtures to help easy production and less pollution. Polycyclic aromatic hydrocarbons (PAHs) are highly intensive and characteristic Raman scatterers. Even small amounts (ppm to ppb scale or less) should be detectable (co-work with IVC-SEP-center). 3) Characterisation of biological and consumer samples, where fluorescence is a problem. Organic molecules, e.g. proteins, nucleic acids (DNA), hormones, phthalates and pigments in the household and other environments should exhibit Raman and resonance Raman spectra with a lot of information on structure and function if only the fluorescence could be avoided. We will try this by a study of insuline in living tissue (distribution, structure and other characterisations). Also we will start on the obvious project of cancer cell characterisation (a co-work with the QUP-center). 4) We are also studying pigments and objects from the Ny Carlsberg Glyptotek. The intention is to set the UV Raman instrument up, and then carry out the subprojects 1) - 4) simultaneously. The ph.d. project will have the complete set of subprojects as its objective, but parts of the work are to be done even without a ph.d.-salary.

Department of Chemistry
Department of Chemical and Biochemical Engineering
Center for Energy Resources Engineering
Period: 01/01/2006 → 01/01/2009
Number of participants: 1
Acronym: UVRS
Project Manager, organisational:
Setofte, Inger (Intern)

Financing sources
Source: Uddannelse, udenlandske offentlige og private
Name of research programme: Uddannelse, udenlandske offentlige og private
Amount: 10,000.00 Danish Kroner
Project

Nye Elektrodematerialer til brændselceller
Department of Chemistry
Period: 01/12/2005 → 19/12/2008
Number of participants: 6
Phd Student: Hjalmarsson, Per (Intern)
Supervisor: Mogensen, Mogens Bjerg (Intern)
Main Supervisor: Fehrmann, Rasmus (Intern)
Examiner: Skaarup, Steen (Intern)
Fleig, Jürgen (Ekstern)
Skou, Eivind Morten (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Risø (Løn)
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 Høgni (Ekstern)
Schüth, Ferdi (Ekstern)

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

Design af Heterogene Katalysatorer
Department of Chemistry
Number of participants: 6
Phd Student: Frey, Anne Mette (Intern)
Supervisor: Christensen, Claus H. (Intern)
Main Supervisor: Fehrmann, Rasmus (Intern)
Examiner: Henriksen, Niels Engholm (Intern)
Nielsen, Michael Brorson (Intern)
Niemantsverdriet, J. W. Hans (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD
**Automotive High Temperature Fuel Cell Membranes**
The automotive application of PEM fuel cells is facing some crucial problems: - the relatively low operating temperatures limiting heat rejection - too small an operating temperature range and - high humidification needs. New types of electrolyte membranes and catalysts offer a solution; their systematic development and testing is the main focus of the effort; along with that work on MEA, entire cells and small scale stacks is foreseen to finally validate the results at a representative level of power. The project combines and exploits the European expertise in the field of advanced polymer membranes in a focused clustered and network type activity. Collaboration with institutes from non EU member states, in particular China, Russia and India, is addressed as well. A steering group with representatives of seven automobile OEMs shall coordinate the project and iteratively focus and guide the developers by specifications and assessment of results.

Department of Chemistry
DaimlerChrysler AG
Centro Ricerche FIAT
Honda R&D Europe (Deutschland) GmbH
Adam Opel AG, International Development Center
Renault France
Toyota Motor Engineering & Manufacturing Europe NV/SA
Volkswagen AG
Bulgarian Academy of Sciences
Centre Nationale de la Recherche Scientifique
Chalmers University of Technology
Consiglio Nazionale delle Ricerche
Deutsches Zentrum Für Luft- und Raumfahrt
Energy Research Centre of the Netherlands
European Institute for Energy Research
Freudenberg FCCT OHG
Gesellschaft für Funktionelle Membranen und Anlagentechnologie mbH
Ilika Technologies Ltd
Johnson Matthey Fuel Cells Ltd
KTH - Royal Institute of Technology
Max Planck Institute
Nuvera Fuel Cells Europe Srl
PEMEAS GmbH
Solvay Solexis S.p.A.
TIMCAL SA
Umicore AG & Co KG
Universita Degli Studi Di Perugia
Helsingin Yliopisto
Lund University
Period: 01/11/2005 → 31/10/2009
Number of participants: 30
Acronym: Autobrane
Contact person:
Erdle, Erich (Ekstern)
Project participant:
Zandiri, Stefania (Ekstern)
Brachmann, Thomas (Ekstern)
Wieser, Christian (Ekstern)
Cornet, Nathalie (Ekstern)
De Colvenaer, Bert (Ekstern)
Hübner, Gerold (Ekstern)
Sinigersky, Veselin (Ekstern)
Jones, Deborah (Ekstern)
Fridell, Erik (Ekstern)
Antonucci, Vincenzo (Ekstern)
Gülzow, Erich (Ekstern)
Wakker, André (Ekstern)
Gautier, Ludmila (Ekstern)
Banhardt, Volker (Ekstern)
Bauer, Bernd (Ekstern)
Hayden, Brian (Ekstern)
Hards, Graham (Ekstern)
Lundblad, Anders Olof (Ekstern)
Klapper, Markus (Ekstern)
Toro, Antonino (Ekstern)
Henschel, Carsten (Ekstern)
Ghielmi, Alessandro (Ekstern)
Bjerrum, Niels J. (Intern)
Li, Qingfeng (Intern)
Corti, Fabrizio (Ekstern)
Zuber, Ralf (Ekstern)
Alberti, Giulio (Ekstern)
Tenhu, Heikki (Ekstern)
Jannasch, Patric (Ekstern)

**Financing sources**
*Source: Forsk. EU - Rammeprogram*
*Name of research programme: Forsk. EU - Rammeprogram*
*Amount: 2,415,000.00 Danish Kroner*

**Financing sources**
*Source: Internal funding (public)*
*Name of research programme: Offentlig finansiering*
*Project: PhD*

### Udvikling af lette materaler til brintlagring

**Department of Chemistry**

**Period:** 01/11/2005 → 01/04/2009  
**Number of participants:** 7  
**Phd Student:**  
Vestbø, Andreas Peter (Intern)  
**Supervisor:**  
Barner, Jens H. Von (Intern)  
Jensen, Jens Oluf (Intern)  
**Main Supervisor:**  
Bjerrum, Niels J. (Intern)  
**Examiner:**  
Jacobsen, Torben (Ekstern)  
Jensen, Torben René (Ekstern)  
Noréus, Dag (Ekstern)  

**Financing sources**
*Source: Forsk. EU - Rammeprogram*
*Name of research programme: Forsk. EU - Rammeprogram*
*Amount: 2,415,000.00 Danish Kroner*

**Financing sources**
*Source: Internal funding (public)*
*Name of research programme: Offentlig finansiering*
*Project: PhD*
Elucidation of Mechanisms for Bio-Hydrogen Production by Computational Methods

Department of Chemistry
Period: 01/10/2005 → 30/09/2010
Number of participants: 6
Phd Student:
Falsig, Hanne (Intern)
Supervisor:
Nørskov, Jens Kehlet (Intern)
Main Supervisor:
Fehrmann, Rasmus (Intern)
Examiner:
Rossmeisl, Jan (Intern)
Grönbeck, Henrik (Ekstern)
Mavrikakis, Manos (Intern)

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

Metal Ammine Complexes as New Hydrogen Storage Materials

Department of Chemistry
Period: 01/10/2005 → 19/12/2008
Number of participants: 6
Phd Student:
Sørensen, Rasmus Zink (Intern)
Supervisor:
Christensen, Claus H. (Intern)
Main Supervisor:
Fehrmann, Rasmus (Intern)
Examiner:
Barner, Jens H. Von (Intern)
Muhler, Martin (Ekstern)
Stoltze, Per (Intern)

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

Studier af metalkatalyserede decarbonyleringer

Department of Chemistry
Period: 15/09/2005 → 01/04/2009
Number of participants: 6
Phd Student:
Taarning, Esben (Intern)
Supervisor:
Christensen, Claus H. (Intern)
Main Supervisor:
Madsen, Robert (Intern)
Examiner:
Fehrmann, Rasmus (Intern)
Andersson, Pher G. (Ekstern)
Begtrup, Mikael (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-lønnet stipendie
Fremstilling af Aminer ved Metalorganiske Reaktioner

Department of Chemistry
Period: 01/09/2005 → 30/01/2009
Number of participants: 5
Phd Student:
Nordstrøm, Lars Ulrik Rubæk (Intern)
Main Supervisor:
Madsen, Robert (Intern)
Examiner:
Tanner, David Ackland (Intern)
Skrydstrup, Troels (Ekstern)
Wärnmark, Kenneth (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Grundforskningsfonden

Fuel and Chemicals from Renewable Alcohols

Department of Chemistry
Period: 01/09/2005 → 19/12/2008
Number of participants: 7
Phd Student:
Hansen, Jeppe Rass (Intern)
Supervisor:
Christensen, Claus H. (Intern)
Madsen, Robert (Intern)
Main Supervisor:
Fehrmann, Rasmus (Intern)
Examiner:
Tanner, David Ackland (Intern)
Chandler, Bert (Ekstern)
Herbst, Konrad (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Grundforskningsfonden

Højtemperatur PEM brændselsceller til energiproduktion og som katalysatorsystem for organiske reaktioner

Department of Chemistry
Period: 01/09/2005 → 16/12/2009
Number of participants: 7
Phd Student:
Cleemann, Lars Nilausen (Intern)
Supervisor:
Bjerrum, Niels J. (Intern)
Li, Qingfeng (Intern)
Main Supervisor:
Petrushina, Irina (Intern)
Examiner:
Steenberg, Thomas (Intern)
Bouzek, Karel (Ekstern)
Skou, Eivind Morten (Ekstern)
Metalorganic reactions with aldehydes and carbohydrates

Department of Chemistry
Period: 01/09/2005 → 25/02/2009
Number of participants: 5
PhD Student:
Monrad, Rune Nygaard (Intern)
Main Supervisor:
Madsen, Robert (Intern)
Examiner:
Nielsen, Thomas Eiland (Intern)
Bols, Mikael (Ekstern)
Thiem, Joachim Erich (Ekstern)

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

Catalytic Conversion of Biofuel

Department of Chemistry
Period: 01/06/2005 → 27/10/2008
Number of participants: 5
PhD Student:
Jørgensen, Betina (Intern)
Main Supervisor:
Fehrmann, Rasmus (Intern)
Examiner:
Makkee, Michiel (Ekstern)
Andersen, Jens (Intern)
Dahl, Søren (Intern)

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

Chemical Design of Functional Nanotube Materials

Department of Chemistry
Period: 01/06/2005 → 25/02/2009
Number of participants: 6
PhD Student:
Egeblad, Kresten (Intern)
Supervisor:
Christensen, Claus H. (Intern)
Main Supervisor:
Fehrmann, Rasmus (Intern)
Examiner:
Ståhl, Kenny (Intern)
Chandler, Bert (Ekstern)
Iversen, Bo Brummerstedt (Ekstern)

Financing sources
Source: Internal funding (public)
Molecular Reaction Dynamics

Department of Chemistry
Period: 01/06/2005 → 31/05/2007
Number of participants: 1

Project Manager, organisational:  
Møller, Klaus Braagaard (Intern)

Financing sources
Source: Forsk. Private danske - Fonde
Name of research programme: Forsk. Private danske - Fonde
Amount: 981,823.00 Danish Kroner

Insulins struktur og kemiske egenskaber i nanoskala og på det enkelte molekyls niveau

Department of Chemistry
Period: 01/05/2005 → 17/06/2010
Number of participants: 7
Phd Student:  
Welinder, Anna Christina (Intern)
Supervisor:  
Steensgaard, Dorte B. (Ekstern)
Zhang, Jingdong (Intern)
Main Supervisor:  
Ulstrup, Jens (Intern)
Examiner:  
Molin, Søren (Intern)
Jensen, Knud Jørgen (Intern)
Nichols, Richard John (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU, Samfinansiering

Organic Synthesis and Biophysical Investigation of Novel Targeted Drug Delivery Systems

Department of Chemistry
Period: 01/03/2005 → 29/08/2008
Number of participants: 7
Phd Student:  
Linderoth, Lars (Intern)
Supervisor:  
Andresen, Thomas Lars (Intern)
Jørgensen, Kent (Intern)
Peters, Günther H.J. (Intern)
Main Supervisor:  
Madsen, Robert (Intern)
Examiner:  
Tanner, David Ackland (Intern)
Thompson, David H. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-lønnet stipendie
Project: PhD
Udvikling af mere effektive og billigere MEA'er til PEM brændselsceller

Department of Chemistry
Polymer Department
Risø National Laboratory for Sustainable Energy
IRD Fuel Cells A/S

Danish Power Systems ApS
Period: 03/02/2005 → 31/01/2008
Number of participants: 5
Project participant:
Li, Qingfeng (Intern)
Andersen, Steen Yde (Ekstern)
Steenberg, Thomas (Ekstern)
Plackett, David (Intern)
Project Manager, organisational:
Bjerrum, Niels J. (Intern)

Financing sources
Source: Forskningsprojekter - Andre ministerier og styrelser
Name of research programme: Forskningsprojekter - Andre ministerier og styrelser
Amount: 2,075,000.00 Danish Kroner

Studies of ferredoxins and dCTP deaminase:dUTPase

Department of Chemistry
Period: 01/02/2005 → 27/06/2008
Number of participants: 7
Phd Student:
Helt, Signe Smedegaard (Intern)
Supervisor:
Ooi, Bee Lean (Intern)
Christensen, Hans Erik Mølager (Intern)
Main Supervisor:
Harris, Pernille (Intern)
Examiner:
Ulstrup, Jens (Intern)
Hagen, Wilfred Raymond (Ekstern)
Henriksen, Anette (Ekstern)

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

Studies on the Total Synthesis of the Natural Products Halichlorine and Pinnaic Acid

Department of Chemistry
Period: 01/02/2005 → 29/08/2008
Number of participants: 5
Phd Student:
Jessing, Mikkel (Intern)
Main Supervisor:
Tanner, David Ackland (Intern)
Examiner:
Madsen, Robert (Intern)
Norrby, Per-Ola (Intern)
Design of functional nanomaterials
To establish a research collaboration encompassing all steps in the development of new functional nanomaterials: design, synthesis, characterization, and testing. The common aim of the proposal is the development of rational design strategies for nano-structured materials.

Department of Physics
Department of Chemistry
Administration
Department of Chemical and Biochemical Engineering
Department of Micro- and Nanotechnology
Risø National Laboratory for Sustainable Energy
Center for Individual Nanoparticle Functionality

Center for Nanoteknologi
Period: 01/01/2005 → 31/12/2008
Number of participants: 19
Project ID: 20195
Project participant:
Jacobsen, Karsten Wedel (Intern)
Chorkendorff, Ib (Intern)
Nielsen, Jane Hvolbæk (Intern)
Horch, Sebastian (Intern)
Schiøtz, Jakob (Intern)
Hansen, Jern Bindslev (Ekstern)
Quaade, Ulrich (Intern)
Christensen, Claus H. (Intern)
Ulstrup, Jens (Intern)
Johannessen, Tue (Intern)
Bøggild, Peter (Intern)
Pedersen, Allan Schröder (Intern)
Linderoth, Søren (Intern)
Mogensen, Mogens (Intern)
Vegge, Tejs (Intern)
Pryds, Nini (Intern)
Henriksen, Peter Vang (Ekstern)
Kuhn, Luise Theil (Intern)

Project Manager, organisational:
Nørskov, Jens Kehlet (Intern)

Financing sources
Source: Forskningsrådene - Andre
Name of research programme: Forskningsrådene - Andre
Amount: 9,290,000.00 Danish Kroner
Project

Etabliering af makromolekylær krystallografisk gruppe
Department of Chemistry
Heterogeneous catalysis for chemical production
Catalysis is one of the technological pillars of modern chemical industry. Catalysis also holds the key to the solution of many environmental and energy problems. The challenge in the field is to devise new methods that can accelerate the development of new catalysts and processes beyond the intuitive trial-and-error approach. It is suggested to form a collaborative program encompassing the whole range from computational design and experimental analysis of model systems to synthesis and testing of new catalysts. The aim of the program is to develop new tools allowing for the rational design of catalysts and catalytic processes for chemical industry and for environmental protection.

Department of Physics
Department of Chemistry
Department of Chemical and Biochemical Engineering
Center for Nanoteknologi
Haldor Topsoe AS
University of Iceland

Petrochallenge – a Competition for High Schools
By combining fun and education, the international PetroChallenge competition encourages high school students in a growing number of countries to take interest in energy resources engineering. CERE has been organizing the national branch of the annual competition since its introduction in Denmark in 2005.

Funded by DONG Energy and Maersk Oil
Center for Energy Resources Engineering

Department of Chemistry
Period: 17/12/2004 → 31/12/2020
Number of participants: 1
Project ID: 50365
Project Manager, academic:
Stenby, Erling Halfdan (Intern)
Dynamik ved grænseflader og i elektroder under drift af elektrolysator og brændselscellesystemer

Department of Chemistry
Period: 01/11/2004 → 25/02/2008
Number of participants: 6
Phd Student:
Nielsen, Jimmi (Intern)
Supervisor:
Mogensen, Mogens Bjerg (Intern)
Main Supervisor:
Jacobsen, Torben (Intern)
Examiner:
Skaarup, Steen (Intern)
Fleig, Jürgen (Ekstern)
Skou, Eivind Morten (Ekstern)

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

Forbedring af Materialer til fast Oxid Brændselsceller

Department of Chemistry
Period: 15/08/2004 → 28/01/2008
Number of participants: 7
Phd Student:
Hauch, Anne (Intern)
Supervisor:
Bilde-Sørensen, Jørgen (Intern)
Mogensen, Mogens Bjerg (Intern)
Main Supervisor:
Jacobsen, Torben (Intern)
Examiner:
Skaarup, Steen (Intern)
Falk, Lena K. L. (Ekstern)
Holtappels, Peter (Intern)

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

Den Molekylære Reaktionsmekanisme for Metalloenzymet Tryptophan-hydroxylase

Department of Chemistry
Period: 01/08/2004 → 14/12/2007
Number of participants: 6
Phd Student:
Windahl, Michael Skovbo (Intern)
Supervisor:
Harris, Pernille (Intern)
Main Supervisor:
Christensen, Hans Erik Mølager (Intern)
Examiner:
Peters, Günther H.J. (Intern)
Bergfors, Terese (Ekstern)
Bollinger Jr., J. Martin (Ekstern)
En ny Peptidmodel med forøget stabilitet

Department of Chemistry
Period: 01/07/2004 → 25/02/2008
Number of participants: 7
Phd Student:
Hosseini, Masood (Intern)
Supervisor:
Dörwald, Florencio Zaragoza (Ekstern)
Tender, Janne Ejrnæs (Intern)
Main Supervisor:
Tanner, David Ackland (Intern)
Examiner:
Madsen, Robert (Intern)
Grøtli, Morten (Ekstern)
Meldal, Morten (Ekstern)

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

Further Improvement and System Integration of High Temperature Polymer Electrolyte Membrane Fuel Cells

The project is devoted to further development of the PEMFC technology based on temperature-resistant polymer membranes for operation above 100°C. The strategic developments of the FURIM are in three steps: (1) improvement of high temperature polymer membranes and related materials; (2) development of technological units including fuel cell stack, hydrocarbon reformer, afterburner and power management system; and (3) integration of the HT-PEMFC stack with these compatible subunits. The advanced features of the integrated power system include high system efficiency, high power density (small size and light weight of the overall system), simple construction and operation, effective cost, high reliability, less maintenance, and better transient response capacities, which are desirable for both automobile and stationary applications.

Department of Chemistry
Volvo Technology Corporation
Norwegian University of Science and Technology
University of Newcastle upon Tyne
Elsam A/S
Danish Power Systems ApS
Case Western Reserve University
University of Stuttgart
Hexion B.V.
IRD Fuel Cells A/S
Period: 01/04/2004 → 31/03/2008
Number of participants: 10
Acronym: FURIM
Project ID: SES6-CT-2004-502782
Project participant:
Ekdunge, Per (Ekstern)
Borresen, Borre (Ekstern)
Scott, Keith (Ekstern)
Henriksen, Niels (Ekstern)
Hennesø, Erik (Ekstern)
Savinell, Robert (Ekstern)
Kerres, Jochen (Ekstern)
Walter, Michael (Ekstern)
Project Manager, organisational:
Bjerrum, Niels J. (Intern)
Yde Andersen, Steen (Ekstern)

Financing sources
Source: Forsk. EU - Rammeprogram
Name of research programme: Forsk. EU - Rammeprogram
Amount: 5,600,000.00 Danish Kroner

Project

Nye Syntesemetoder fra kulhydrater

Department of Chemistry
Period: 01/03/2004 → 28/09/2007
Number of participants: 5
Phd Student:
Hansen, Flemming Gundorph (Intern)
Main Supervisor:
Madsen, Robert (Intern)
Examiner:
Tanner, David Ackland (Intern)
Ellervik, Ulf C. (Ekstern)
Jensen, Knud Jørgen (Intern)

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

Studies of chemical and physical properties of strontium compounds
Synthesis and characterisation of metalorganic compounds of strontium. The purified salt were applied to controlled release studies of strontium in rat serum and in rat urine. Results patented.

Department of Chemistry
Osteologix A/S
Period: 26/02/2004 → 31/12/2005
Number of participants: 2
Project ID: 40258
Contact person:
Andersen, Jens (Intern)
Project participant:
Andersen, Jens (Intern)

Financing sources
Source: Indtægtsdækket virksomhed UK 90
Name of research programme: Indtægtsdækket virksomhed UK 90
Amount: 50,000.00 Danish Kroner
Project

Studies of chemical and physical properties of strontium compounds
Synthesis and characterisation of metalorganic compounds of strontium. The purified salt were applied to controlled release studies of strontium in rat serum and in rat urine. Results patented.

Department of Chemistry
Osteologix A/S
Period: 26/02/2004 → 31/12/2004
Number of participants: 2
Project ID: 40258
Contact person: Andersen, Jens (Intern)
Project participant: Andersen, Jens (Intern)

**Financing sources**
Source: Indtægtsdækket virksomhed UK 90
Name of research programme: Indtægtsdækket virksomhed UK 90
Amount: 10,000.00 Danish Kroner

**Project**

*Studies of chemical and physical properties of strontium compounds: Controlled Release Composition Containing a Strontium Salt*

Synthesis and characterisation of metallorganic compounds of strontium. The purified salt were applied to controlled release studies of strontium in rat serum and in rat urine. Results patented.

Department of Chemistry
Symbion Science Park
Nordic Bone A/S
Osteologix A/S
Period: 26/02/2004 → 31/12/2005
Number of participants: 2
Project ID: 40258
Contact person: Andersen, Jens (Intern)
Project participant: Andersen, Jens (Intern)

**Financing sources**
Source: Indtægtsdækket virksomhed UK 90
Name of research programme: Indtægtsdækket virksomhed UK 90
Amount: 10,000.00 Danish Kroner

**Project**

*Mechanistic Investigation of Organometallic Addition Reactions*

Department of Chemistry
Period: 01/02/2004 → 25/04/2007
Number of participants: 6
Phd Student: Ahlquist, Mårten Sten Gösta (Intern)
Supervisor: Tanner, David Ackland (Intern)
Main Supervisor: Norrby, Per-Ola (Intern)
Examiner: Madsen, Robert (Intern)
Andersson, Pher G. (Ekstern)
Bendix, Jesper (Ekstern)

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

Bioelectrochemical and Scanning Probe Studies of Oligonucleotides on single-crystal gold electrodes
Department of Chemistry
Period: 01/01/2004 → 01/05/2007
Number of participants: 6
Phd Student:
Grubb, Mikala (Intern)
Supervisor:
Wackerbarth, Hainer (Intern)
Main Supervisor:
Ulstrup, Jens (Intern)
Examiner:
Henriksen, Niels Engholm (Intern)
Jensen, Knud Jørgen (Intern)
Nichols, Richard John (Intern)

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

Hejtemperature PEM brandselscelle
Department of Chemistry
Tech-wise A/S
Danish Power Systems ApS
IRD Fuel Cells A/S
Period: 01/01/2004 → 30/09/2006
Number of participants: 4
Project ID: 4760
Project participant:
Henriksen, Niels (Ekstern)
Hennesø, Erik (Ekstern)
Yde Andersen, Steen (Ekstern)
Project Manager, organisational:
Bjerrum, Niels J. (Intern)

Financing sources
Source: Forskningsrådene - Andre
Name of research programme: Forskningsrådene - Andre
Amount: 1,850,000.00 Danish Kroner
Project

Novel Electrochemically Activated Catalysts and Processes
Department of Chemistry
Period: 01/01/2004 → 31/12/2006
Number of participants: 2
Project ID: 40244
Project participant:
Petrushina, Irina (Intern)
Project Manager, organisational:
Bjerrum, Niels J. (Intern)

Financing sources
Source: Forskningsrådene - SNF
Name of research programme: Forskningsrådene - STVF
Amount: 222,000.00 Danish Kroner
Project
Synthesis, characterization and applications of polymer membranes for high temperature fuel cells
The project deals with novel materials for an advanced polymer membrane fuel cell system, which produces electricity and heat from natural gas, biomass or other environmentally friendly fuels. The fuel cell system operates at about 200°C with a high CO-tolerance (at least 30,000 ppm). This high CO tolerance makes it possible for the fuel cell system to use reformate hydrogen obtained directly from reforming of various types of fuel. The system can therefore be used for both mobile and stationary applications with a high energy efficiency and considerably reduced emissions, compared to the present technology. As the key requisite for this technology, temperature-resisting polymers will be synthesized, membranes of the polymers will be fabricated and functionalised for creating proton conductivity. Electrochemical and fuel cell tests and other physical chemical characterizations will be carried out. Correlations between the materials structures and performances will be established. Evaluation of the materials and fabrication processes will be made.

Department of Chemistry
University of Copenhagen
Period: 01/01/2004 → 31/12/2006
Number of participants: 2
Project ID: 2058-03-0005
Project Manager, organisational: Bjerrum, Niels J. (Intern)
Begtrup, Micheal (Ekstern)

Financing sources
Source: Forskningsrådene - STVF
Name of research programme: Forskningsrådene - STVF
Amount: 1,000,000.00 Danish Kroner
Project

Udvikling af 2 kW naturgasreformere for høj- og lavtemperatur PEM-brændselsceller
Department of Chemistry
Danish Gas Technology Centre A/S
IRD Fuel Cells A/S
Danfoss A/S
Danish Power Systems ApS
DONG Energy A/S
Aalborg University
Period: 01/01/2004 → 30/09/2006
Number of participants: 7
Project ID: 33030-0021
Contact person:
Bjerrum, Niels J. (Intern)
Project participant:
Yde Andersen, Steen (Ekstern)
Balslev, Per (Ekstern)
Steenberg, Thomas (Ekstern)
Pedersen, Aksel Hauge (Ekstern)
Kær, Søren Knudsen (Ekstern)
Project Manager, organisational:
Wit, Jan de (Ekstern)

Financing sources
Source: Forskningsprojekter - Miljø- og Energiministeriet
Name of research programme: Forskningsprojekter - Miljø- og Energiministeriet
Amount: 930,000.00 Danish Kroner
Project

Undersøgelse af interaktioner mellemlectiner og sukkerarer, vha. AFM-mikrobiologi og molekylær dynamiske stimuleringer
Department of Chemistry
Period: 01/01/2004 → 26/10/2007
Number of participants: 7
Phd Student:
Nygaard, Thomas Pedersen (Intern)
Supervisor:
Hansen, Flemming Yssing (Intern)
Jensen, Morten Østergaard (Intern)
Main Supervisor:
Peters, Günther H.J. (Intern)
Examiner:
Møller, Klaus Braagaard (Intern)
Schiøtt, Hanne Birgti (Ekstern)
Åqvist, Johan L. G. (Ekstern)
Financing sources
Source: Internal funding (public)
Name of research programme: DTU-lønnet stipendie
Project: PhD

X-ray investigation of pharmaceuticals

Department of Chemistry
Ferring Pharmaceuticals A/S
Period: 01/01/2004 → 31/12/2007
Number of participants: 2
Project ID: 40256
Contact person:
Hammar, Emma (Ekstern)
Project Manager, organisational:
Ståhl, Kenny (Intern)

Financing sources
Source: Indtægtsdækket virksomhed UK 90
Name of research programme: Indtægtsdækket virksomhed UK 90
Amount: 118,250.00 Danish Kroner

X-ray synchrotron studies
DANSYNC is paid by SNF and supports synchrotron radiation based research through covering of materials, development costs and travelling expenses.

Department of Chemistry
Niels Bohr Institute
Period: 01/01/2004 → 31/12/2007
Number of participants: 2
Project ID: 40257
Contact person:
Ståhl, Kenny (Intern)
Project Manager, organisational:
Feidenhans'l, Robert (Ekstern)

Financing sources
Source: Forskningsrådene - SNF
Name of research programme: Forskningsrådene - STVF
Amount: 126,000.00 Danish Kroner

Stereoselektiv Syntese af Biologisk Aktive Stoffer og Naturprodukter fra Kulhydrater

Department of Chemistry
Number of participants: 6
Phd Student:
Fanefjord, Mette (Intern)
Supervisor:
Madsen, Robert (Intern)
Main Supervisor:
Lundt, Inge (Intern)
Examiner:
Gotfredsen, Charlotte Held (Intern)
Nielsen, Poul (Ekstern)
Wrodnigg, Tanja M. (Ekstern)

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

Syntese af Naturstoffer fra Kulhydrater
Department of Chemistry
Period: 01/10/2003 → 03/09/2007
Number of participants: 5
Phd Student:
Pipper, Charlotte Bressen (Intern)
Main Supervisor:
Madsen, Robert (Intern)
Examiner:
Lundt, Inge (Intern)
Pedersen, Erik Bjerregaard (Ekstern)
Stütz, Arnold (Intern)

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

Synthesis, characterization and photocatalytic properties of Ti- and V-containing materials with different porosity
Department of Chemistry
Number of participants: 5
Phd Student:
Kustova, Marina (Intern)
Main Supervisor:
Christensen, Claus H. (Intern)
Examiner:
Stähl, Kenny (Intern)
Corma, Avelino (Ekstern)
Herbst, Konrad (Ekstern)

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

Development of methodologies for determination of trace-level concentrations of element by atomic spectrometry via on-line pretreatment procedures
Department of Chemistry
Number of participants: 7
Phd Student:
Long, Xiangbao (Intern)
Supervisor:
Andersen, Jens (Intern)
Miró, Manuel (Ekstern)
Main Supervisor:
Hansen, Elo Harald (Intern)
Examiner:
Heydorn, Kaj (Intern)
Karlberg, Bo Ingemar (Ekstern)
Larsen, Erik Huusfeldt (Intern)

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

### Mechanistic Investigation of Metal-Catalyzed Formation of Three-Membered Rings

Department of Chemistry
Number of participants: 2
Phd Student:
Kringelum, Henriette (Intern)
Main Supervisor:
Norrby, Per-Ola (Intern)

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

### Lysopsamling i farvestofknyttede block copolymerer

Department of Chemistry
Period: 01/08/2003 → 23/10/2006
Number of participants: 6
Phd Student:
Nielsen, Kim Troensegaard (Intern)
Supervisor:
Krebs, Frederik C (Intern)
Main Supervisor:
Harris, Pernille (Intern)
Examiner:
Thorup, Niels (Intern)
Higgins, Simon J. (Ekstern)
Spanget-Larsen, Jens (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Risø (Løn)
Project: PhD

### Synthesis of Biologically Active Natural Products

Department of Chemistry
Number of participants: 5
Phd Student:
Molekyldynamiske simuleringer af Lipidmembraners Vekselvirkning med Membranaktive Enzymer

Department of Chemistry
Period: 01/04/2003 → 28/08/2006
Number of participants: 7
Phd Student:
Sonne, Jacob (Intern)
Supervisor:
Hansen, Flemming Yssing (Intern)
Jensen, Morten Østergaard (Intern)
Main Supervisor:
Peters, Günther H.J. (Intern)
Examiner:
Møller, Klaus Braagaard (Intern)
Ipsen, John Hjorth (Intern)
Marrink, Siewert Jan (Ekstern)

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

New Methodology for the Medium Scale Solid-Phase Synthesis of Small Drug Molecules

Department of Chemistry
Period: 01/03/2003 → 12/06/2006
Number of participants: 6
Phd Student:
Rudbeck, Hans Christian (Ekstern)
Supervisor:
Dancer, Robert J. (Ekstern)
Main Supervisor:
Tanner, David Ackland (Intern)
Examiner:
Gotfredsen, Charlotte Held (Intern)
Jensen, Knud Jørgen (Intern)
Vedsø, Per (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: ErhvervsPhD-ordningen VTU
Project: PhD

Selective Homogeneous Catalysis in Asymmetric Synthesis

Department of Chemistry
Period: 01/03/2003 → 08/05/2006
Number of participants: 6
Phd Student:
Fristrup, Peter (Intern)
Supervisor:
Tanner, David Ackland (Intern)
Main Supervisor:
Norrby, Per-Ola (Intern)
Examiner:
Christensen, Claus H. (Intern)
Goodman, Jonathan M. (Ekstern)
Jørgensen, Karl Anker (Ekstern)

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

Røntgenkarakterisering af Nanostrukturerede Materialer med Specielt Henblik på Indflydelsen af Partikelstørrelse og Defekter

Department of Chemistry
Period: 01/02/2003 → 15/05/2008
Number of participants: 6
Phd Student:
Oddershede, Jette (Intern)
Supervisor:
Jiang, Jianzhong (Intern)
Main Supervisor:
Ståhl, Kenny (Intern)
Examiner:
Hagen, Anke (Intern)
Feidenhans'l, Robert Krarup (Intern)
Guagliardi, Antonietta (Ekstern)

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

New Metal Hydrides for Energy Storage

Department of Chemistry
Department of Physics
Institute for Energy Technology
Stockholm University
University of Oslo
Lithuanian Energy Institute
Helsinki University of Technology
Period: 01/01/2003 → 31/12/2006
Number of participants: 8
Project ID: 62-02
Project participant:
Jensen, Jens Oluf (Intern)
Noréus, Dag (Ekstern)
Fjellvåg, Helmer (Ekstern)
Noréus, Dag (Ekstern)
Opgradering af SMART rntgendiffraktometer til et system, der kan bruges til målinger på krystaller af både små molekyler og proteiner

Department of Chemistry  
Period: 01/01/2003 → 31/12/2003  
Number of participants: 1  
Project Manager, organisational: Harris, Pernille (Intern)

Financing sources  
Source: Forskningsrådene - SNF  
Name of research programme: Forskningsrådene - STVF  
Amount: 1,332,762.00 Danish Kroner

Mechanistic Investigation of Metal-Catalyzed formation of Three-Memberedrings

Department of Chemistry  
Period: 01/11/2002 → 30/04/2003  
Number of participants: 2  
Phd Student: Olsen, Per Tetzschner (Intern)  
Main Supervisor: Norrby, Per-Ola (Intern)

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

Egenskaber af perovskitter med varierende A/B-forhold

Department of Chemistry  
Period: 01/10/2002 → 24/01/2006  
Number of participants: 8  
Phd Student: Søgaard, Martin (Intern)  
Supervisor: Hendriksen, Peter Vang (Intern)  
Mogensen, Mogens Bjerg (Intern)  
Poulsen, Finn Willy (Intern)  
Main Supervisor: Jacobsen, Torben (Intern)  
Examiner: Skaarup, Steen (Intern)  
Bouwmeester, Henny J. M. (Ekstern)  
Grande, Tor (Ekstern)

Financing sources
**Sammenhænge mellem Strukturer og Ydeevne for Sofc Anoder**

Department of Chemistry  
Period: 01/10/2002 → 24/01/2006  
Number of participants: 7  
Phd Student:  
Klemensø, Trine (Intern)  
Supervisor:  
Larsen, Jørgen Gutzon (Ekstern)  
Mogensen, Mogens Bjerg (Intern)  
Main Supervisor:  
Jacobsen, Torben (Intern)  
Examiner:  
Skaarup, Steen (Intern)  
Ivers-Tiffée, Ellen (Ekstern)  
Skou, Eivind Morten (Ekstern)

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Risø (Løn)  
Project: PhD

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**Sintering Studies of Supported Metal Catalysts by in Situ TEM**

Department of Chemistry  
Period: 01/10/2002 → 28/08/2006  
Number of participants: 8  
Phd Student:  
Hansen, Thomas Willum (Intern)  
Supervisor:  
Datye, Abhaya K. (Ekstern)  
Hansen, Poul Lenvig (Ekstern)  
Helveg, Stig (Ekstern)  
Main Supervisor:  
Ståhl, Kenny (Intern)  
Examiner:  
Horch, Sebastian (Intern)  
Crozier, Peter A. (Ekstern)  
Malm, Jan-Olle (Ekstern)

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: ErhvervsPhD-ordningen VTU  
Project: PhD

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**Total Synthesis of Zoanthamine Alkaloids**

Department of Chemistry  
Period: 01/09/2002 → 22/12/2005  
Number of participants: 5  
Phd Student:  
Hjelmgaard, Thomas (Intern)  
Main Supervisor:  
Tanner, David Ackland (Intern)  
Examiner:  
Madsen, Robert (Intern)
Dörwald, Florencio Zaragoza (Ekstern)
Skrydstrup, Troels (Ekstern)

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

**Fremstilling af biologisk vigtige naturstoffer fra kulhydrater**
Department of Chemistry
Period: 01/08/2002 → 20/12/2005
Number of participants: 5
Phd Student:
Lauritsen, Anne (Intern)
Main Supervisor:
Madsen, Robert (Intern)
Examiner:
Lundt, Inge (Intern)
Gothelf, Kurt Vesterager (Ekstern)
Nielsen, Poul (Ekstern)

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

**Metal/Hydrogen elektroders kinetik på faststofelektrolytter**
Department of Chemistry
Period: 01/06/2002 → 30/09/2005
Number of participants: 8
Phd Student:
Høgh, Jens Valdemar Thorvald (Intern)
Supervisor:
Chorkendorff, Ib (Intern)
Hansen, Karin Vels (Intern)
Mogensen, Mogens Bjerg (Intern)
Main Supervisor:
Jacobsen, Torben (Intern)
Examiner:
Skaarup, Steen (Intern)
Brongersma, Hidde Herman (Ekstern)
Skou, Eivind Morten (Ekstern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Risø (Løn)
Project: PhD

**Molekylær Dynamik og Kemisk Kinetik**
Department of Chemistry
Period: 01/06/2002 → 31/05/2005
Number of participants: 1
Project Manager, organisational:
Møller, Klaus Braagaard (Intern)

**Financing sources**
Source: Forskningsrådene - SNF
Name of research programme: Forskningsrådene - STVF
**Stereoselektiv syntese af biologisk aktive stoffer/naturprodukter med kulhydrater som chirale udgangsstoffer**

Department of Chemistry  
Period: 01/03/2002 → 01/06/2005  
Number of participants: 5  
Phd Student:  
Bøjstrup, Marie (Intern)  
Main Supervisor:  
Lundt, Inge (Intern)  
Examiner:  
Tanner, David Ackland (Intern)  
Bols, Mikael (Ekstern)  
Stütz, Arnold (Intern)

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

**1,5-Anhydro-D-fructose as a chiral building block**

Department of Chemistry  
Period: 01/02/2002 → 22/12/2005  
Number of participants: 5  
Phd Student:  
Andreassen, Mikkel (Intern)  
Main Supervisor:  
Lundt, Inge (Intern)  
Examiner:  
Jensen, Søren Rosendal (Intern)  
Bols, Mikael (Ekstern)  
Pedersen, Erik Bjerregaard (Ekstern)

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Anden EU-finansiering  
Project: PhD

**Kædeforlængelse af kulhydrater med metalorganiske reagenser**

Department of Chemistry  
Period: 01/02/2002 → 09/12/2005  
Number of participants: 5  
Phd Student:  
Palmelund, Anders (Intern)  
Main Supervisor:  
Madsen, Robert (Intern)  
Examiner:  
Norrby, Per-Ola (Intern)  
Begtrup, Mikael (Ekstern)  
Konradsson, Peter Gunnar (Ekstern)

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Forskningsrådsstipendium  
Project: PhD
Metalkatalyserede reaktioner på det anomere center i kulhydrater

Department of Chemistry
Period: 01/02/2002 → 30/09/2005
Number of participants: 4
Phd Student:
Keinicke, Lise Edelmann (Intern)
Main Supervisor:
Madsen, Robert (Intern)
Examiner:
Gottfredsen, Charlotte Held (Intern)
Hindsgaul, Ole (Ekstern)

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

Syntase af naturstoffer

Department of Chemistry
Period: 01/02/2002 → 26/08/2005
Number of participants: 4
Phd Student:
Håkansson, Anders Eckart (Intern)
Main Supervisor:
Madsen, Robert (Intern)
Examiner:
Ruhland, Thomas (Ekstern)
Skrydstrup, Troels (Ekstern)

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

Materialeproblemer i affaldskedler

Department of Chemistry
Department of Management Engineering
Elsam A/S
Energi E2 A/S
Barbcock & Wilcox Vølund A/S
FLS Miljø A/S

Mineral Development International
Period: 01/01/2002 → 31/12/2006
Number of participants: 8
Project ID: PSO no. 4104
Project participant:
Bjerrum, Niels J. (Intern)
Cappeln, Frederik Vilhelm (Intern)
Larsen, Ole Hede (Ekstern)
Tiedje, Niels (Ekstern)
Jensen, Jørgen Peter (Ekstern)
Matthiesen, Henrik Dam (Ekstern)
Iversen, Steen B. (Ekstern)
Frederiksen, Jens (Ekstern)
Organic Synthesis using Solid-Supported Reagents

Department of Chemistry
Period: 01/11/2001 → 28/03/2006
Number of participants: 6
Phd Student:
Hansen, Anne-Lene Lauesgaard (Ekstern)
Supervisor:
Murray, Anthony (Ekstern)
Main Supervisor:
Tanner, David Ackland (Intern)
Examiner:
Norrby, Per-Ola (Intern)
Begtrup, Mikael (Ekstern)
Nielsen, John (Intern)

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

Heterogeneous Catalysts for Asymmetric Epoxidation Reactions

Department of Chemistry
Period: 01/10/2001 → 04/03/2005
Number of participants: 7
Phd Student:
Hasselriis, Peter (Intern)
Supervisor:
Christensen, Claus H. (Intern)
Hagen, Anke (Intern)
Main Supervisor:
Fehrmann, Rasmus (Intern)
Examiner:
Tanner, David Ackland (Intern)
Herbst, Konrad (Ekstern)
Roessner, Frank (Ekstern)

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

Asymmetric solid-phase synthesis and applications in combinatorial chemistry

Department of Chemistry
Period: 01/09/2001 → 01/09/2001
Number of participants: 2
Phd Student:
Severinsen, Rune Eg (Intern)
Main Supervisor:
Nielsen, John (Intern)

Financing sources
Source: Internal funding (public)
Synthesis of New Quorum Sensing Inhibitors

Department of Chemistry  
Period: 01/09/2001 → 04/04/2005  
Number of participants: 6  
Phd Student: Persson, Tobias (Ekstern)  
Supervisor: Nielsen, John (Intern)  
Main Supervisor: Tanner, David Ackland (Intern)  
Examiner: Lundt, Inge (Intern) Bols, Mikael (Ekstern) Breinbauer, Rolf (Ekstern)

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

Stereocontrolled synthesis of Lyngbyatoxinm A pharmacologically Active Natural product

Department of Chemistry  
Period: 01/05/2001 → 22/01/2007  
Number of participants: 5  
Phd Student: Vital, Paulo (Intern)  
Main Supervisor: Tanner, David Ackland (Intern)  
Examiner: Madsen, Robert (Intern) Craig, Donald (Ekstern) Dörwald, Florencio Zaragoza (Ekstern)

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

De Novo Organic Synthesis abd Biophysical Investigation of Novel Liposome Systems in relation to Drug Delivery

Department of Chemistry  
Period: 01/04/2001 → 17/03/2005  
Number of participants: 9  
Phd Student: Andresen, Thomas Lars (Intern)  
Supervisor: Begtrup, Mikael (Ekstern) Jørgensen, Kent (Intern) Lundt, Inge (Intern) Mouritsen, Ole G. (Intern)  
Main Supervisor: Madsen, Robert (Intern)  
Examiner: Peters, Günther H.J. (Intern) Barenholz, Yechezkel (Ekstern)
**Wengel, Jesper (Ekstern)**

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

**Nanostructured Catalysts**
Department of Chemistry
Period: 15/03/2001 → 03/06/2005
Number of participants: 6
Phd Student: Andreasen, Jens Wenzel (Intern)
Supervisor: Feidenhans'l, Robert Krarup (Intern)
Main Supervisor: Ståhl, Kenny (Intern)
Examiner: Gerward, Leif (Intern)
Benedetti, Alvise (Ekstern)
Grunwaldt, Jan-Dierk (Intern)

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

**Studies on The Total Synthesis of Halichlorine and Pinnalc Acid**
Department of Chemistry
Period: 01/03/2001 → 10/09/2004
Number of participants: 5
Phd Student: Kvaerner, Lisbet (Intern)
Main Supervisor: Tanner, David Ackland (Intern)
Examiner: Madsen, Robert (Intern)
Paterson, Ian (Ekstern)
Skrydstrup, Troels (Ekstern)

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

**Advanced Methanol Fuel Cell Systems**
The project aims at developing materials and technologies for an advanced methanol fuel cell system for vehicle propulsion. The system is an integration of a methanol reformer, a catalytic burner, and a fuel cell stack operational at temperatures around 200°C.

Department of Chemistry
Volvo Technology Corporation
Norwegian University of Science and Technology
Statoil ASA
Period: 01/02/2001 → 31/08/2005
Number of participants: 4
Acronym: AMFC
Project ID: ENK5-CT-2000-00323
Contact person:
Bjerrum, Niels J. (Intern)
Project participant:
Tunold, Radar (Ekstern)
Klov, Kår (Ekstern)
Project Manager, organisational:
Ekdunge, Per (Ekstern)

Financing sources
Source: Forsk. EU - Rammeprogram
Name of research programme: Forsk. EU - Rammeprogram
Amount: 6,800,000.00 Danish Kroner
Project

Smøremidler og smøremekanismer ved plastisk formgivning af metalliske materialer
Department of Chemistry
Period: 01/02/2001 → 07/07/2005
Number of participants: 7
Phd Student:
Nilsson, Morten Sixten (Intern)
Supervisor:
Christensen, Erik (Intern)
Petrushina, Irina (Intern)
Main Supervisor:
Bjerrum, Niels J. (Intern)
Examiner:
Gillesberg, Bo (Intern)
Skou, Eivind Morten (Ekstern)
Steenberg, Thomas (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Ansat eksternt CAMP
Project: PhD

Termoelasticitet og Dynamik af Membraner og Makromolekyler
Department of Chemistry
Period: 01/02/2001 → 23/08/2004
Number of participants: 6
Phd Student:
Henriksen, Jonas Rosager (Intern)
Supervisor:
Ipsen, John Hjorth (Intern)
Main Supervisor:
Hansen, Flemming Yssing (Intern)
Examiner:
Henriksen, Niels Engholm (Intern)
Meleard, Philippe (Ekstern)
Mitov, Marin (Ekstern)

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

High Temperature Polymer Methanol Fuel Cell,
Department of Chemistry
New products from Starch-derived 1,5-Anhydro-D-fructose

The novel sugar 1,5-anhydro-D-fructose (AF) will be produced on an industrial scale from starch by a biocatalytic process with -1,4-glucan lyase. Starch is a renewable, environment-friendly, and cheap raw material which belongs to the major agriculture products of the EU. Therefore, AF is an abundant starting material for versatile use whose bulk price will be similar to other starch sugars. Although AF itself has a market potential as a functional ingredient and a calory-free sweetener, its market potential will be significantly expanded if AF is also used as a building block for the manufacturing of high-value added products. In this respect AF is a promising chemical synthon, because it possesses a fixed pyranoid ring structure and a prochiral center at carbon 2. A pre-requisite for developing new product lines from AF, is an easy access to AF and its economic production. Up to date, this is hampered by the biocatalyst, -1,4-glucan lyase, whose catalytic properties have to be improved by protein engineering for an ideal industrial performance. Commercialization of AF and derivatives thereof is envisaged by traditional and start-up bioindustries, that participate in this transdisciplinary project. Major goals are to improve AF production with advanced biotechnological methods, and to develop new reaction routes for the synthesis of multiple high value-added products from AF. Possible food or medical applications require to study the bioactivity of the respective products.
Punching and stamping of stainless steel is characterised as tribologically difficult due to galling caused by the brittle oxides and the large affinity of the base material to pick-up on the tool surface resulting in scoring of subsequently passing work piece surface. Until recently, the only lubricants able to impede galling in severe deep drawing, stretch forming and ironing operations were chlorinated paraffin oils, which are expected to be abandoned in near future due to environmental problems. In a national Danish research programme, 1994-99, two new lubricant systems have been developed as substitutes to chlorinated paraffin oils. Testing of these environmentally harmless lubricants under controlled laboratory conditions has shown very promising results and so has initial industrial tests at Danfoss, Grundfos and Volvo among others. In the present research programme "Industrial punching/blanking and sheet metal forming – lubricants, mechanisms of lubrication and environmental aspects" running from 2000-2003 the development and testing of lubrication systems will be further studied in a co-operative project between Institut for Kemi, DTU, Institut for Produktion, DTU (in the following named IPT), Danfoss, Grundfos, RM Rich. Müller, Esti Chem and Houghton Danmark. Objectives The objective of the present project is to develop a general methodology for determination of the limits of lubrication in sheet metal forming of stainless steel. Furthermore development and testing of tailor-made surface topographies improving the resistance to lubricant film breakdown will be studied.

A general Synthetic route to octa/decahydroquinolines via ring-closing metathesis (RCM)

Department of Chemistry
Period: 01/09/2000 → 09/12/2005
Number of participants: 5
Phd Student: Nolsøe, Jens Mortansson Jelstrup (Intern)
Main Supervisor: Tanner, David Ackland (Intern)
Examiner:
Norrby, Per-Ola (Intern)
Bols, Mikael (Ekstern)
Vedsø, Per (Ekstern)

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

Kombinatoriske Biblioteker af Naturstofderivater
Department of Chemistry
Period: 01/09/2000 → 26/01/2004
Number of participants: 6
Phd Student:
Laursen, Jane B. (Intern)
Supervisor:
Nielsen, John (Intern)
Main Supervisor:
Tanner, David Ackland (Intern)
Examiner:
Norrby, Per-Ola (Intern)
Skrydstrup, Troels (Ekstern)
Yli-Kauhaluoma, Jari Tapani (Ekstern)

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

Development of new Catalytic Asymmetric Reactions Simple and Economic Synthesis of Chiral Building proces
Department of Chemistry
Period: 01/08/2000 → 25/03/2004
Number of participants: 6
Phd Student:
Seitzberg, Jimmi Gerner (Intern)
Supervisor:
Johannsen, Mogens (Intern)
Main Supervisor:
Tanner, David Ackland (Intern)
Examiner:
Madsen, Robert (Intern)
Andersson, Pher G. (Ekstern)
Dörwald, Florencio Zaragoza (Ekstern)

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

Avancerede overfladebehandlinger
Department of Chemistry
Period: 01/04/2000 → 14/10/2003
Number of participants: 6
Phd Student:
Precht Noyé, Pernille (Intern)
Supervisor:
Barner, Jens H. Von (Intern)
Screening and Evaluation of Synthetic Carbohydrate Receptors
Department of Chemistry
Period: 01/04/2000 → 20/11/2003
Number of participants: 7
Phd Student:
Ridderberg, Signe Marit (Intern)
Supervisor:
Heeg-Jensen, Thomas (Ekstern)
Østergaard, Søren Duus (Ekstern)
Main Supervisor:
Lundt, Inge (Intern)
Examiner:
Jensen, Søren Rosendal (Intern)
Bøg-Hansen, Torkild Christian (Ekstern)
Norrild, Jens Chr. (Intern)
Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Development of new catalytic reactions - simple and economic synthesis of chiral compounds
Department of Chemistry
Period: 01/03/2000 → 27/08/2003
Number of participants: 6
Phd Student:
Jensen, Jakob Feldthusen (Intern)
Supervisor:
Johannsen, Mogens (Intern)
Main Supervisor:
Tanner, David Ackland (Intern)
Examiner:
Madsen, Robert (Intern)
Bäckvall, Jan-Erling (Ekstern)
Skrydstrup, Troels (Ekstern)
Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsfinansiering
Project: PhD

Metalorgisk kemi på kulhydrater
Department of Chemistry
Period: 01/03/2000 → 10/11/2004
Number of participants: 5
Phd Student:
Advanced Surface Treatments
The project deals with surface modifications of steel and titanium based materials to improve corrosion and abrasion resistance. The scope is to provide the fundamental and technical data necessary to develop new CVD (chemical vapour deposition) and electrochemical based processes. The elements to be used in surface coatings are mainly titanium, niobium, zirconium, boron, carbon and nitrogen - either in the pure form or in combination such as alloys or borides, nitrides and carbides. These materials show in general high corrosion resistance and a good biocompatibility. The borides, carbides and nitrides are materials with large hardness. Our approach to the formation of the mentioned surfaces are for the main part entirely new and unexplored. In the choice of reaction media we will try to minimize possible environmental and health hazards. (Danish Ministry of Research)
Copper and Zinc complex chemistry
Complex chemistry of various copper and zinc compounds is being studied by a multiple instrumental approach.

Department of Chemistry

Department of Chemistry
Period: 01/01/2000 → 01/01/2001
Number of participants: 2
Project participant:
Ulstrup, Jens (Intern)
Project Manager, organisational:
Berg, Rolf W. (Intern)

Exploiting flow injection/sequential injection on-line separation and preconcentration schemes for determination of ultra-trace levels of metals by means of ETAAS and ICPMS

Department of Chemistry
Period: 01/10/1999 → 06/12/2002
Number of participants: 5
Phd Student:
Wang, Jianhua (Intern)
Main Supervisor:
Hansen, Elo Harald (Intern)
Examiner:
Andersen, Jens (Intern)
Adams, Freddy (Ekstern)
Larsen, Erik Huusfeldt (Intern)

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

Carboproteins - Carbohydrates as templates for proteinmodels

Department of Chemistry
Period: 01/09/1999 → 06/01/2003
Number of participants: 6
Phd Student:
Brask, Jesper (Intern)
Supervisor:
Jensen, Knud Jørgen (Intern)
Main Supervisor:
Nielsen, John (Intern)
Examiner:
Nørby, Per-Ola (Intern)
Høeg-Jensen, Thomas (Ekstern)
Meldal, Morten (Ekstern)

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

Elucidation of Functional Groups in Pectin
Pectin is a polysaccharide found in many fruits such as apples and citrus fruits. Danisco-Cultor A/S has a dominating role for production of pectin as a functional food ingredient. In order to obtain better control of properties of pectin in existing applications or to add new application areas it is necessary to strengthen the fundamental research of the molecular structure of pectin. Danisco-Cultor has obtained fundings (centerkontrakt) from the Danish research councils to a collaboration with DTU (Department of Organic Chemistry and Department of Biotechnology) and Southern University of Denmark, Odense, for this purpose. The current project aims at developing methods for esterification of raw-pectin (possibly for industrial uses), and smaller pectin-fragments, delivered by Danisco. Analytical tools for determining the degree of
Esteification has to be developed, including using NMR-spectroscopy. Other selective modifications of the carboxylic groups within pectin should be investigated. The modified pectin (fragments) might induce different enzymatic degradation and thus lead to new properties of pectin. Another part of the synthetic project, headed by associate professor Robert Madsen, aims at synthesise defined building blocks of smaller protected fragments of di-tri- and tetra-saccharides of the galacturonic acids, which is the monomeric carbohydrate building the core structure of pectin. This strategy would lead to the final goal, namely to prepare tailor-made smaller pectin fragments with specific structure/substitution pattern, used for evaluation of mass spectrometric analytical methods by other partners in the project.

Department of Organic Chemistry
Department of Chemistry
Danisco-Cultor
Period: 01/09/1999 → 31/08/2002
Number of participants: 6
Project participant:
Rosenbohm, Christoph (Intern)
Madsen, Robert (Intern)
Clausen, Mads Hartvig (Intern)
Christensen, Tove (Ekstern)
Mikkelsen, Jørn Dalgård (Ekstern)
Project Manager, organisational:
Lundt, Inge (Intern)

Financing sources
Source: Unknown
Name of research programme: Ukendt
Amount: 1,654,000.00 Danish Kroner

Elektrokemi og in situ scanning tunnel mikroskopi af biologisk betydningsfulde overgangsmetalkomplekser

Department of Chemistry
Period: 01/06/1999 → 14/03/2003
Number of participants: 5
Phd Student:
Hansen, Allan Glargaard (Intern)
Supervisor:
Boisen, Anja (Intern)
Main Supervisor:
Ulstrup, Jens (Intern)
Examiner:
Quaade, Ulrich (Intern)
Raiteri, Robert (Ekstern)

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

Kemisk syntese af oligosakkarider indeholdt i pectin

Department of Chemistry
Period: 01/06/1999 → 28/02/2003
Number of participants: 6
Phd Student:
Clausen, Mads Hartvig (Intern)
Supervisor:
Lundt, Inge (Intern)
Main Supervisor:
Madsen, Robert (Intern)
Examiner:
Tanner, David Ackland (Intern)
Bock, Klaus (Ekstern)
Wengel, Jesper (Ekstern)

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

Metalorganiske Reaktioner på Kulhydrater
Department of Chemistry
Period: 01/06/1999 → 31/03/2003
Number of participants: 5
Phd Student:
Skaanderup, Philip Robert (Intern)
Main Supervisor:
Madsen, Robert (Intern)
Examiner:
Lundt, Inge (Intern)
Bols, Mikael (Ekstern)
Frejd, Torbjørn (Ekstern)

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

Mobilitet af kationer i oxid-ionledere
Department of Chemistry
Period: 01/05/1999 → 02/01/2001
Number of participants: 2
Phd Student:
Hinnum, Benjamin (Intern)
Main Supervisor:
Jacobsen, Torben (Intern)

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

Bifasisk katalyse
Department of Chemistry
Period: 01/04/1999 → 20/09/2002
Number of participants: 6
Phd Student:
Riisager, Anders (Intern)
Supervisor:
Hjortkjær, Jes (Intern)
Main Supervisor:
Fehrmann, Rasmus (Intern)
Examiner:
Tanner, David Ackland (Intern)
Andersson, Carlaxel (Ekstern)
Christensen, Claus H. (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Centerfinansieret
Development of a Method for On-line Measurements of High Temperature Corrosion
The aim of the project is to develop a method for on-line measurements of high temperature corrosion. It is the idea to use the method in order to keep corrosion under surveillance under various types of operation in existing power plants. For this purpose an electrochemical noise probe will be designed and tested at Masnedø Power Station near Vordingborg – a biomass fired plant constructed in 1996 which only uses straw as fuel.

Department of Chemistry
Elkraft A.m.b.A.
Elsam A/S
Period: 01/04/1999 → 31/03/2002
Number of participants: 3
Project participant:
Cappeln, Frederik Vilhelm (Intern)
Petrushina, Irina (Intern)
Project Manager, organisational:
Bjerrum, Niels J. (Intern)
Project

Alkenyltin Chemistry: Method Development and Applications in Organic Synthesis
Department of Chemistry
Period: 01/03/1999 → 16/07/2002
Number of participants: 6
Phd Student:
Nielsen, Thomas Eiland (Intern)
Supervisor:
Kjær, Anders (Intern)
Main Supervisor:
Tanner, David Ackland (Intern)
Examiner:
Madsen, Robert (Intern)
Frejd, Torbjörn (Ekstern)
Skrydstrup, Troels (Ekstern)

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

Elektronisk inducerede organiske reaktioner
Department of Chemistry
Period: 01/02/1999 → 21/10/2002
Number of participants: 6
Phd Student:
Hansen, Bo Stenhuus (Intern)
Supervisor:
Nielsen, Merete Folmer (Ekstern)
Main Supervisor:
Jacobsen, Torben (Intern)
Examiner:
Skaarup, Steen (Intern)
Daasbjerg, Kim (Ekstern)
Skou, Eivind Morten (Ekstern)

Financing sources
Kemisk syntese af legeringskatalysatorer

Department of Chemistry
Period: 01/02/1999 → 16/07/2002
Number of participants: 7
Phd Student:
Barfod, Rasmus Gottrup (Intern)
Supervisor:
Chorkendorff, Ib (Intern)
Teunissen, Hermann (Ekstern)
Main Supervisor:
Fehrmann, Rasmus (Intern)
Examiner:
Henriksen, Niels Engholm (Intern)
Nielsen, Michael Brorson (Intern)
Grunwaldt, Jan-Dierk (Intern)

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

Kontaktering af keramiske materialer i fastoxid-brændselscelle

Department of Chemistry
Period: 01/02/1999 → 28/05/2002
Number of participants: 6
Phd Student:
Koch, Søren (Intern)
Supervisor:
Mogensen, Mogens Bjerg (Intern)
Main Supervisor:
Jacobsen, Torben (Intern)
Examiner:
Skaarup, Steen (Intern)
Nisancioglu, Kemal (Ekstern)
Skou, Eivind Morten (Ekstern)

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

Molecular Dynamics Simulations of Proteins, Biomembrane Systems, and Interfaces

Department of Chemistry
Period: 01/02/1999 → 16/09/2002
Number of participants: 6
Phd Student:
Jensen, Morten Østergaard (Intern)
Supervisor:
Peters, Günther H.J. (Intern)
Main Supervisor:
Mouritsen, Ole G. (Intern)
Examiner:
Hansen, Flemming Yssing (Intern)
Raman Spectroscopy of Lightening Elements
Laser Raman spectroscopy can be used to nondestructively measure molecular species that are found in pressurized tungsten-halogen bulbs. Reactions are studied in experimental bulbs filled bromine containing molecules, inert gasses (Kr or Ar) and rare earth salts. The molecular composition is studied versus accumulated burning time. Compounds HBr, CO, and SiF4, etc. are expected to form in the bulb. Raman spectroscopy can also be used to identify solid deposits (e.g. W oxides) on the inside surface of the glass envelope. The total pressure in the bulb can be measured nondestructively by Rayleigh scattering.
Reliability improvements for co-combustion plants
Program under The European Coal and Steel Community (EU).

Department of Chemistry
Cranfield University
Elkraft Power Company Ltd
Elsam Project Ltd

UTT Manufacturing Technology
Period: 01/02/1999 → 31/01/2002
Number of participants: 3
Project participant:
Cappeln, Frederik Vilhelm (Intern)
Petrushina, Irina (Intern)

Project Manager, organisational:
Bjerrum, Niels J. (Intern)

Lipase-lipid interactions
Molecular dynamics simulations (MD) have become a powerful tool for studying the structure and dynamics of biologically important molecules such as lipases. A vast amount of theoretical and experimental work have appeared in the literature indicating that these enzymes act on a lipid interface (e.g., micelles, monolayers or bilayers). In the present project, simulations are applied to study the effect of a lipid interface on the protein dynamics and hence on the activation of the enzyme. In particular, the effect of the lipid charge distribution on the adsorption of the enzyme and activation will be addressed.

Department of Chemistry

Combinatorial synthesis of quorum sensing inhibitors
This program embrace the generation of targeted combinatorial libraries aimed against intercellular communication for applications within e.g. food preservation and infectious disease area. Using solid-phase synthesis and combinatorial chemistry, modulators of quorum sensing is developed.

Department of Organic Chemistry
Department of Microbiology
National Food Institute
Department of Systems Biology
Department of Chemistry

Period: 01/01/1999 → 31/12/2002
Number of participants: 5
Project participant:
Olsen, Jacob Alsbæk (Intern)
Molin, Søren (Intern)
Givskov, Michael Christian (Intern)
Gram, Lone (Intern)

Project Manager, organisational:
Nielsen, John (Intern)
Design and Synthesis of Protein Kinase Inhibitors by Combinatorial Chemistry
New modulators of protein kinase activity are designed and synthesized using combinatorial chemistry and high-throughput synthesis.

Department of Organic Chemistry
Department of Chemistry
Period: 01/01/1999 → 31/12/2001
Number of participants: 3
Project participant:
Olsen, Jacob Alsbæk (Intern)
Issinger, Olaf-Georg (Ekstern)
Project Manager, organisational:
Nielsen, John (Intern)

Financing sources
Source: Unknown
Name of research programme: Ukendt
Amount: 600,000.00 Danish Kroner

Development of high temperature stable friction materials
Erhvers-ph.d. i samarbejde med OBTEC A/S og Afdeling for Materialeforskning, Risø

Department of Chemistry
Period: 01/01/1999 → 31/12/2001
Number of participants: 1
Project Manager, organisational:
Høj, Jakob Weiland (Intern)

Development of high temperature stable friction materials

Department of Chemistry
Period: 01/01/1999 → 14/02/2002
Number of participants: 8
Phd Student:
Ramousse, Severine (Intern)
Supervisor:
Petrushina, Irina (Intern)
Sørensen, Ole Toft (Intern)
Valentin, Jesper (Ekstern)
Main Supervisor:
Bjerrum, Niels J. (Intern)
Examiner:
Andersen, Birger Kr (Intern)
Hjuler, Hans Aage (Intern)
Skou, Eivind Morten (Ekstern)

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

Electronic Structure Calculations
Detailed calculations of molecular electronic structures with emphasis on bonding, spin-density, catalytic activity, geometry, and spectroscopic properties. Targets for the investigations are small organic and inorganic molecules as well as transition metal complexes. Recent studies include the interaction between ammonia and sulfur dioxide (triplet states), the pyrosulfate ion (geometry and vibrations), and some analogous compounds having the same bridging structure. The calculations apply SCF, MCSCF, CI and perturbation methods using the program systems Gaussian-98 and MOLCAS
version 4 as well as locally developed programs. The project is partly financed by a grant from The Danish Natural Sciences Research Council (SNF).

Department of Chemistry

Department of Chemistry
Period: 01/01/1999 → 31/12/1999
Number of participants: 1
Project Manager, organisational:
Johansen, Helge (Intern)

Encaged Metal Complexes
At a simplistic level, metal complexes encapsulated in e.g. a zeolite may be considered as inorganic analogues of natural metallo-enzymes, with the zeolite framework representing a rigid protein mantle. The present project is focused on the question: How does the structure and reactivity of a metal complex species confined in a porous silica framework compare with those of the same species in a protein matrix?

Department of Chemistry

Department of Chemistry
Period: 01/01/1999 → 31/12/2000
Number of participants: 2
Project participant:
Christensen, Hans Erik Mølager (Intern)
Project Manager, organisational:
Bagger, Sven (Intern)

Industrial punching and ironning - lubrication mechanisms and environmental aspects (ISOPS)
"Center Contract". Danish Ministry of Research.

Department of Chemistry

Department of Manufacturing Engineering
Danfoss A/S
Esti Chem A/S
Houghton Denmark A/S
Rich. Müller A/S
Period: 01/01/1999 → 31/12/2002
Number of participants: 4
Project participant:
Petrushina, Irina (Intern)
Li, Qingfeng (Intern)
Christensen, Erik (Intern)
Project Manager, organisational:
Bjerrum, Niels J. (Intern)

Metal hydride storage tank for hydrogen vehicle
The aim of the project is to develop and produce a metal hydride based hydrogen storage tank for demonstration purposes. The tank will be used (1) in a hydrogen car with combustion engine reconstructed by "Nordvestjysk Folkecenter for Vedvarende Energi" and (2) in a car with fuel cells from IRD A/S in cooperation with Fiat.

Department of Chemistry

Risø National Laboratory for Sustainable Energy
IRD A/S
Period: 01/01/1999 → 30/06/2000
Number of participants: 3
Project participant:
Microwave irradiation to expedite and facilitate organic reactions

Microwave irradiation to expedite and facilitate organic reactions: Application in solid-phase and combinatorial synthesis.

Department of Organic Chemistry

Phase Equilibria and Thermodynamic Properties of Biological Polymers.

The research activities aim towards developing methods for predicting a range of thermodynamic properties based on fundamental chemistry. Earlier experience has shown that in the molecular structure there is a key to many properties, and that information about larger molecules can often be retrieved from studies of smaller systems. 1. Thermodynamic properties of carbohydrates using QSPR (Quantitative Structure Property Relationships). In QSPR modelling the physical or thermodynamic property of interest is correlated to a series of structural properties. Presently the project is concerned with small organic substances which contain similar functional groups as saccharides, like alkanes, alcohols and polyols. 2. Measurements and modelling of phase equilibria of oligo- and polysaccharides in aqueous solution. Molecular interactions will be studied with experiments and molecular modelling in order to gain a better understanding of how these substances behave in an aqueous environment.

Production and distribution of power and heat

Department of Chemistry

Financing sources

Source: Unknown
Name of research programme: Uknown
Amount: 3,000,000.00 Danish Kroner

Project
Electrochemical Promotion of Catalytic Reactions
The project is concerned with the study of the effect of electrochemical disturbances on the activity and selectivity of catalytic systems. The project builds upon the network, experience and scientific results obtained by Department of Chemistry (DTU) in the field of electrochemistry, fuel cells and catalysis. With regard to this project, recent discoveries concerning the effect of non-Faradaic electrochemical promotion of liquid-phase catalytic reactions (SO2 oxidation) are of special interest. The project consists of two main tasks: 1. Electrochemical promotion of the catalytic conversion of the polluting emissions from combustion engines. 2. Electrochemical promotion of the catalytic oxidation of methane to methanol. (1. ICAT project).

Department of Chemistry
Period: 08/12/1998 → 31/12/2002
Number of participants: 5
Project participant:
Petrushina, Irina (Intern)
Cappeln, Frederik Vilhelm (Intern)
Gang, Xiao (Intern)
Qingfeng, Li (Ekstern)
Project Manager, organisational:
Bjerrum, Niels J. (Intern)

Dielektriske polymerer til aktuatorer
Department of Chemistry
Period: 01/12/1998 → 04/01/2002
Number of participants: 6
Phd Student:
Kofod, Guggi (Intern)
Supervisor:
Sommer-Larsen, Peter (Intern)
Main Supervisor:
Skaarup, Steen (Intern)
Examiner:
Lyngaae-Jørgensen, Jørgen (Intern)
Davies, Geoffrey R. (Ekstern)
Schaumburg, Kjeld (Ekstern)

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

Syntese af kulhydratbaserede enyner og ringslutning til carbocykler
Department of Chemistry
Period: 01/12/1998 → 28/05/2002
Number of participants: 5
Phd Student:
Poulsen, Carina Storm (Intern)
Main Supervisor:
Madsen, Robert (Intern)
Examiner:
Lundt, Inge (Intern)
Meldal, Morten (Ekstern)
Vedsø, Per (Ekstern)

Financing sources
Source: Internal funding (public)
**Combinatorial carbohydrate chemistry**

Department of Organic Chemistry

Department of Chemistry

Period: 01/09/1998 → 31/12/2001

Number of participants: 2

Project participant:

Andersen, Kim (Ekstern)

Project Manager, organisational:

Jensen, Knud Jørgen (Intern)

**Rational design, synthesis and characterization of metalloproteins containing cuboidal molybdenum clusters**

Department of Chemistry

Period: 01/08/1998 → 05/02/2002

Number of participants: 6

Phd Student:

Caspersen, Mikael Bjerg (Intern)

Supervisor:

Christensen, Hans Erik Mølager (Intern)

Main Supervisor:

Ulstrup, Jens (Intern)

Examiner:

Thorup, Niels (Intern)

Bjerrum, Morten Jannik (Ekstern)

Nielsen, Michael Brorson (Intern)

**Financing sources**

Source: Internal funding (public)

**Stereospecific glycosylation by intramolecular base-catalyzed transglycosylation**

Department of Chemistry

Period: 01/08/1998 → 05/02/2002

Number of participants: 6

Phd Student:

Petersen, Lars (Intern)

Supervisor:

Jensen, Knud Jørgen (Intern)

Main Supervisor:

Nielsen, John (Intern)

Examiner:

Tanner, David Ackland (Intern)

Bols, Mikael (Ekstern)

Skrydstrup, Troels (Ekstern)

**Financing sources**

Source: Internal funding (public)

**Studier af in situ SPM af elektrokristallisation og adsorberede proteiner**
Department of Chemistry
Period: 01/08/1998 → 15/11/2001
Number of participants: 6
Phd Student: Nielsen, Jens Ulrik (Intern)
Supervisor: Ulstrup, Jens (Intern)
Main Supervisor: Andersen, Jens (Intern)
Examiner: Welinder, Karen G. (Intern)
Nichols, Richard John (Intern)
Quaade, Ulrich (Intern)

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

Lavtemperatursintring af Pb(Zr,Ti)O3

Department of Chemistry
Period: 01/06/1998 → 08/03/2002
Number of participants: 7
Phd Student: Ravn Nielsen, Eva (Intern)
Supervisor: Poulsen, Finn Willy (Intern)
Ringgaard, Erling (Intern)
Main Supervisor: Ståhl, Kenny (Intern)
Examiner: Jacobsen, Torben (Ekstern)
Damjanovic, Dragan (Ekstern)
Grahl-Madsen, Laila (Ekstern)

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

Omdannelse af methan til methanol

Department of Chemistry
Period: 01/05/1998 → 20/09/2002
Number of participants: 6
Phd Student: Birch, Henning (Intern)
Supervisor: Gang, Xiao (Intern)
Main Supervisor: Bjerrum, Niels J. (Intern)
Examiner: Andersen, Birger Kr (Intern)
Larsen, Leif Erik (Ekstern)
Steenberg, Thomas (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsstipendium
Advanced Solid Polymer Fuel Cells for Operation at Temperatures up to 200oC (ASPEC)

As a clean and efficient technology fuel cells are expected to provide a practical form of power generation. Among these solid polymer fuel cells (SPFC) using e.g. perfluorosulfonic acid polymer membrane (naftion,µ) have been receiving more and more attention due to their promise as a power generator for both stationary and transportation applications. The operational temperature is limited to be below 100 oC at atmospheric pressure since the presence of water is necessary. The low temperature results in a low catalytic activity at the electrodes (and hence slow kinetics) and strong effect of fuel impurity poisoning. As a consequence neither methanol nor hydrogen from reforming of hydrocarbons can be used. The requirement of high purity hydrogen as the fuel not only increases operation cost but also limits the application of the SPFC. To overcome these problems the present project aims to develop materials and technologies for an advanced high temperature solid polymer fuel cell (HTSPFC) stack operating at 150 ¡V 200oC with hydrogen from methane or methanol steam reforming (containing 2-3 % CO) as fuel. This will avoid problems associated with hydrogen storage and make the new technology promising in stationary on-site power generation plants and especially for transportation applications. (JOULE programme (EU))
Main Supervisor:
Fehrmann, Rasmus (Intern)
Examiner:
Livbjerg, Hans (Intern)
Bostrup, Ole (Ekstern)
Østvold, Terje (Ekstern)

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

Rationel design, syntese og karakterisering af katalytisk relevante artificielle metalloproteiner
Department of Chemistry
Period: 01/02/1998 → 08/02/2002
Number of participants: 2
Phd Student:
Hansen, Anne Merete (Intern)
Main Supervisor:
Ulstrup, Jens (Intern)

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

Stereokontrolleret etablering af C-C bindinger i kulhydratderivater
Department of Chemistry
Period: 01/02/1998 → 16/07/2002
Number of participants: 5
Phd Student:
Wagner, Sussi Holstein (Intern)
Main Supervisor:
Lundt, Inge (Intern)
Examiner:
Nielsen, John (Intern)
Pedersen, Erik Bjerregaard (Ekstern)
Stütz, Arnold (Intern)

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

Syntese og karakterisering af DeNOx katalysatorer
Department of Chemistry
Period: 01/02/1998 → 19/04/2002
Number of participants: 6
Phd Student:
Mattsson, Rikke Christina (Intern)
Supervisor:
Gabrielsson, Pär (Ekstern)
Main Supervisor:
Fehrmann, Rasmus (Intern)
Examiner:
Ståhl, Kenny (Intern)
Christensen, Claus H. (Intern)
Odenbrand, Ingemar (Ekstern)

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

**Synthesis of anti-inflammatory aminothiazoles**
Regioselective synthesis of aminothiazoles, with the aim of finding inhibitors of inflammatory mediators such as leukotrienes and cytokines.

Department of Organic Chemistry

**Department of Chemistry**

**Period:** 01/02/1998 → 01/01/9999

**Number of participants:** 3

**Project participant:**
- Björkling, Fredrik (Ekstern)

**Project Manager, organisational:**
- Tanner, David Ackland (Intern)
- Norrby, Per-Ola (Intern)

**Financing sources**
- Unknown
  **Amount:** 605,900.00 Danish Kroner
- Unknown
  **Amount:** 323,000.00 Danish Kroner

**Project**

**Calculation of the Electronic Structures of Molecules**
Detailed calculations of molecular electronic structures with emphasis on bonding, spin-density, catalytic activity, geometry, and spectroscopic properties. Targets for the investigations are small organic and inorganic molecules as well as transition metal complexes. Recent studies include (Cu(H2O)6)2+, the interaction between ammonia and sulfur dioxide (triplet states), the pyrosulfate ion (geometry and vibrations), and some compounds containing NO-radicals (spin-density and ESR). The calculations apply SCF, MCSCF, CI and perturbation methods using the program systems Gaussian-94 and MOLCAS versions 3 and 4 as well as locally developed programs. The project is partly financed by a grant from The Danish Natural Sciences Research Council (SNF).

Department of Chemistry

**Department of Chemistry**

**Period:** 01/01/1998 → 31/12/1998

**Number of participants:** 1

**Project Manager, organisational:**
- Johansen, Helge (Intern)

**Project**

**Lubrication Mechanisms and Lubricants for Cold Forging and Sheetforming of Stainless Steel**
As an alternative to machining, bulk and sheet forming of stainless steel has large potential in Danish industry producing pumps, equipment for dairy and other victual products etc. This concerns especially the two groups of forming processes "cold forging" and "deep drawing". Due to the high flow stress and heavy strain hardening, however, the tribological conditions are very severe. New tribologic tests are developed, to make up a series of tests ranging from laboratory tests to full scale production tests. New lubricants are evaluated with respect to their environmental safety. The new type of lubricants for sheet forming of stainless steel developed during the previous MUP2-project (annual reports 1996-97) have been further improved, and tested on a variety of different types of steel and other metals as well as of different geometries of specimens. This work has been carried out in close collaboration with the other project partners. Furthermore, an electrolytic process for applying coatings of zinc-calcium-phosphate on stainless steel previously developed, has been further improved. These coatings are used in combination with sodium stearate as lubricants for cold forging of stainless steel. Work concerning problems of upscaling this coating process has been carried out, including methods for process control etc. The possibility of preparing other types of coatings in a similar way (metal oxides and hydroxides) has also been investigated.
Methane concentration and isotopic composition in soil

Methane concentration in soil gas is measured by gas-chromatography in various depths. The isotopic composition (d(13C)) is determined by isotope ratio mass spectrometry. The results are analyzed in a model describing the soil as a methane sink with a narrow layer of methane producing material.

Synthesis of Nanostructured Materials by High-Energy Ball Milling

The field of nanostructured materials is in a rapid development in many disciplines, e.g. condensed matter physics and materials science. Several techniques have been applied for sample preparation, for example, gas condensation, sputtering, electrodeposition, and thermochemical methods. One of the methods that has received significant attention is mechanical attrition: the high-energy ball milling of single or multicomponent powders. In this year, we successfully synthesised nanometer-sized ZnFe2O4, NiFe2O4, CuFe2O4, nanoalloying in Fe2O3-SnO2, Fe-Cu and mechanochemical reactions in Fe-S.
A Monte Carlo Study on the effects of excluded volume interactions on the scattering from block copolymer micelles and branched polymers

Department of Chemistry
Period: 01/12/1997 → 12/07/2001
Number of participants: 6
Phd Student: Svaneborg, Carsten (Intern)
Supervisor: Pedersen, Jan Skov (Intern)
Main Supervisor: Mouritsen, Ole G. (Intern)
Examiner: Hansen, Flemming Yssing (Intern)
Freire, Juan J. (Ekstern)
Jonsson, Bo (Ekstern)

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

Chemistry and structure-activity relationship of substituted aminothiazoles and related heterocycles with anti-inflammatory activity

Department of Chemistry
Period: 01/12/1997 → 04/03/2002
Number of participants: 7
Phd Student: Hansen, Thomas (Intern)
Supervisor: Bjørkeling, Frederik (Ekstern)
Norrby, Per-Ola (Intern)
Main Supervisor: Tanner, David Ackland (Intern)
Examiner: Pedersen, Erik Bjerregaard (Ekstern)
Bywater, Robert Paul (Ekstern)
Vedsø, Per (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Erhvervsforskerordningen
Development of air metal hydride battery (AMHBAT)

Development of air metal hydride battery (AMHBAT). The aim of the project is to develop a rechargeable air hydride battery to be used in electric vehicles (EV). The operating principle of an air metal hydride battery is rather simple: Water is split into hydrogen and oxygen as the battery is charged. Oxygen is released to the atmosphere and hydrogen is stored in the negative electrode which is made of a hydrogen storage alloy similar to those used in nickel metal hydride batteries. On discharge the process is reversed, and stored hydrogen recombines with atmospheric oxygen to form water. The air hydride battery has been studied since 1988 at Helsinki University of Technology (HUT) and the state of the art is a prototype batteries (24 V, 360 W) made by HUT and the Finnish company Hydrocell. The project involves 5 European universities and 6 industries. It is Supported by the European Community (JOULE, fourth framework programme).

Department of Chemistry
Aalto University
KTH - Royal Institute of Technology
Höganäs AB
Norsk Hydro
Stockholm University
Norwegian University of Science and Technology
GfE Metalle und Materialien
OY Hydrocell Ltd
NiMe Hydrid AB
Elcat Electric Vehicles

Period: 01/12/1997 → 30/11/2000
Number of participants: 2

Project participant:
Jensen, Jens Oluf (Intern)

Project Manager, organisational:
Bjerrum, Niels J. (Intern)

Elektrokatalytisk gasrensning

Department of Chemistry
Period: 01/12/1997 → 25/05/2001
Number of participants: 6

Phd Student:
Kammer Hansen, Kent (Intern)

Supervisor:
Zachau-Christiansen, Birgit (Intern)

Main Supervisor:
Skaarup, Steen (Intern)

Examiner:
Mogensen, Mogens Bjerg (Intern)
Kilner, John (Ekstern)
Koksbang, René (Ekstern)

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

New methods for stereoselective synthesis via desymmetrisation reactions and kinetic resolution
Studies in asymmetric witting-type reactions: Methods development and applications in total synthesis

Investigations of the substrate specificity of protein tyrosine phosphatases

New techniques in Solid-phase Oligosaccharide Synthesis
Fastfase og kombinatorisk syntese af naturstoffer eller andre lead compound

Department of Chemistry
Period: 01/09/1997 → 21/11/2001
Number of participants: 5
Phd Student:
Olsen, Jacob Alsbæk (Intern)
Main Supervisor:
Nielsen, John (Intern)
Examiner:
Johannsen, Mogens (Intern)
Begtrup, Mikael (Ekstern)
Bräse, Stefan (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsstip.-SU, Eksp
Project: PhD

Lipaseaktivitet i relation til lipide substraters fysiske egenskaber

Department of Chemistry
Period: 01/08/1997 → 21/11/2001
Number of participants: 5
Phd Student:
Høyrup, Lise Pernille Kristine (Intern)
Main Supervisor:
Mouritsen, Ole G. (Intern)
Examiner:
Hansen, Flemming Yssing (Intern)
Kinnunen, Paavo J. K. (Ekstern)
Petersen, Steffen B. (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-Su Stipendium, Eksperiment
Project: PhD

Anvendelse af mikro-Ramansprektroskopi til analyse af fasellige vægte i multikomponentsystemer

Department of Chemistry
Period: 01/07/1997 → 27/03/2001
Number of participants: 2
Phd Student:
Hansen, Susanne Brunsgaard (Intern)
Main Supervisor:
Berg, Rolf W. (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Blandet Finansiering-SU
Project: PhD
Raman Spectroscopy Analysis of Phase Equilibria
Phase Equilibria in multicomponent systems, e.g. in fuels, oil and gasses, are studied by Raman and IR spectroscopy. The project is a ph.d. project for Susanne Brunsgaard Hansen, supported by The National Oil and Gas Company of Denmark, The Nordic Energy Research Program and The Danish Technical Research Council.

Department of Chemistry
Department of Chemical and Biochemical Engineering
Center for Energy Resources Engineering
DONG Energy A/S
Nordiske Energiforskningsprogram
Period: 01/07/1997 → 30/01/2001
Number of participants: 3
Project participant:
Hansen, Susanne Brunsgaard (Intern)
Stenby, Erling Halfdan (Intern)
Project Manager, organisational:
Berg, Rolf W. (Intern)

Financing sources
Source: Unknown
Name of research programme: Ukenndt
Amount: 648,000.00 Danish Kroner
Source: Unknown
Name of research programme: Ukenndt
Amount: 274,485.00 Danish Kroner
Source: Unknown
Name of research programme: Ukenndt
Amount: 100,000.00 Danish Kroner
Source: Unknown
Name of research programme: Ukenndt
Amount: 150,000.00 Danish Kroner

Strukturelle og elektriske egenskaber af perovskitter
Department of Chemistry
Period: 01/07/1997 → 05/07/2001
Number of participants: 6
Phd Student:
Hansen, Jesper Rømer (Intern)
Supervisor:
Poulsen, Finn Willy (Intern)
Main Supervisor:
Jacobsen, Torben (Intern)
Examiner:
Skaarup, Steen (Intern)
Bouwmeester, H. J. M. (Ekstern)
Skou, Eivind Morten (Ekstern)

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

Water
An effort is made to develop a new force field for water in all phases. It is based on ab initio calculations on water clusters; electron diffraction in the gas phase; microwave, Raman and IR spectroscopy in gaseous and condensed phases; x-ray and neutron diffraction of ice.
**Metalloprotein Research**

Expression of recombinant metalloproteins: Our studies have concerned development of expression systems for the production of heterologous metalloproteins in bacteria. This includes systems with appropriate removable purification-tags, as well as systems for post translation modifications. We have successfully developed expression systems for a number of important classes of metalloproteins e.g. di-heme cytochromes, blue copper proteins and iron-sulphur proteins. Rational Design of Artificial Metalloproteins: Rational metalloprotein design is an approach for testing general theories of metalloprotein chemistry through the creation and examination of new structures and functions, as well as creation of new catalytic systems. We have successfully synthesised a new class of metalloproteins, for which a patent application has been filed. We are in the process of exploring the chemical, physical and spectroscopic properties of this intriguing new class of metalloproteins. These projects are partly financed by grants from The Danish Technical Research Council and The Danish Natural Science Research Council.

**Financing sources**

- Source: Unknown
  - Name of research programme: Ukendt
    - Amount: 3,000,000.00 Danish Kroner
  - Name of research programme: Ukendt
    - Amount: 102,000.00 Danish Kroner
  - Name of research programme: Ukendt
    - Amount: 493,500.00 Danish Kroner
  - Name of research programme: Ukendt
    - Amount: 422,405.00 Danish Kroner
  - Name of research programme: Ukendt
    - Amount: 50,742.00 Danish Kroner
  - Name of research programme: Ukendt
    - Amount: 100,000.00 Danish Kroner
  - Name of research programme: Ukendt
    - Amount: 271,397.00 Danish Kroner

**Zinc-Mediated Fragmentation of w-Iodoglycosides : A New Route to Functionalized Carbocycles.**

Department of Chemistry

- Period: 01/05/1997 → 18/10/2000
- Number of participants: 3
- Phd Student: Hyldtoft, Lene (Intern)
Developement, optimisation, and application of ICP-SFMS methods for the measurements of isotope ratios

Department of Chemistry
Period: 01/04/1997 → 05/01/2000
Number of participants: 3
Phd Student: Sturup, Stefan (Intern)
Main Supervisor: Hansen, Elo Harald (Intern)
Examiner: Andersen, Jens (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsstip.-SU, Eksp
Project: PhD

Azakulhydrater

Department of Chemistry
Period: 01/03/1997 → 19/11/2001
Number of participants: 5
Phd Student: Malle, Birgitte Mølholm (Intern)
Main Supervisor: Lundt, Inge (Intern)
Examiner: Jensen, Søren Rosendal (Intern)
Bols, Mikael (Ekstern)
Pedersen, Erik Bjerregaard (Ekstern)

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

Phase Equilibria by Molecular Mechanics

A method for predicting interaction parameters used in phase equilibrium calculations has been developed, in which molecular mechanics calculations of the interaction energies between pairs of molecules in the solution of interest is carried out. The method has been used to calculate the vapor-liquid equilibrium for non-polar as well as polar organic solutions with and without hydrogen bonds, and for polymer solutions. The method has also been extended to predict solid-liquid equilibria of carbohydrates in aqueous solution. The interaction energy is calculated as the difference between the potential energy of a pair of molecules isolated in space and the potential energies of the individual molecules. Three such interaction energies must be determined in order to calculate at pair of interaction parameters for a binary mixture; one between unlike molecules and two between like molecules. Two molecules can be oriented in many different ways relative to each other, and several conformers of each molecule may also be possible. Sampling the conformational space of two isolated molecules in a reasonable manner is therefore a complex problem. It is carried out as a Monte Carlo search combined with energy minimization. A molecular mechanics description of the system consists of a series of inter-atomic potentials for non-bonded interactions, as well as internal degrees of freedom. We have found that it is possible to study inter-molecular interactions on a microscopic scale, and to use these results in order to gain insight into the behavior on a macroscopic scale.
Department of Chemistry
Period: 01/03/1997 → 31/12/2000
Number of participants: 4
Project participant:
Rasmussen, Kjeld (Intern)
Rasmussen, Peter (Ekstern)
Klein, Roger A. (Ekstern)
Project Manager, organisational:
Jonsdottir, Svava Osk (Intern)

AFM Studier af Lipidmembraners
Department of Chemistry
Period: 01/02/1997 → 18/07/2000
Number of participants: 4
Phd Student:
Nielsen, Lars Kildemark (Intern)
Supervisor:
Bjørnholm, Thomas (Intern)
Main Supervisor:
Mouritsen, Ole G. (Intern)
Examiner:
Grey, Francois (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-Su Stipendium, Eksperiment
Project: PhD

FIA on-line opkoncentreringsteknikker og specieringsprocedurer
Department of Chemistry
Period: 01/02/1997 → 09/11/2000
Number of participants: 3
Phd Student:
Nielsen, Steffen (Intern)
Main Supervisor:
Hansen, Elo Harald (Intern)
Examiner:
Mosbæk, Hans (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsstip.-SU, Eksp
Project: PhD

Metalloproteiners totalsyntese
Department of Chemistry
Period: 01/02/1997 → 18/09/2000
Number of participants: 3
Phd Student:
Jensen, Thomas Jon (Intern)
Main Supervisor:
Ulstrup, Jens (Intern)
Examiner:
Hammershøj, Anders (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-Su Stipendium, Eksperiment
Project: PhD

**New Handles for Solid-Phase Synthesis**
Department of Organic Chemistry
Department of Chemistry
Period: 01/02/1997 → 31/12/2001
Number of participants: 2
Project participant:
Christensen, Jørn Erik Berril (Intern)
Project Manager, organisational:
Jensen, Knud Jørgen (Intern)

**Transition Metal Complexes**
Many enzymes have been recognised to contain transition metal ions in their active sites. The crystal structure of several transition metal complexes has been determined. The research is carried out in cooperation with chemist at the University of Odense.

Department of Chemistry
University of Southern Denmark
Period: 01/01/1997 → 31/12/2002
Number of participants: 2
Project participant:
McKenzie, Christine (Ekstern)
Project Manager, organisational:
Søtofte, Inger (Intern)

**Ceramic Membranes for Hot Gas Separation**
Department of Chemistry
Department of Chemistry
Haldor Topsoe AS
Number of participants: 3
Project participant:
Tranto, Janne (Intern)
Klem, Connie Janet (Intern)
Project Manager, organisational:
Høj, Jakob Weiland (Intern)

**Financing sources**
Source: Unknown
Name of research programme: Ukendt
Amount: 450,000.00 Danish Kroner

**Deterioration of collagen in parchment**
Manuscripts of parchment belong to the most valuable objects of European cultural heritage. With the increasing air pollution the deterioration of parchment is severely accelerated, and within a few decades, an enormous demand for conservation and restauration is expected. A research group with participants from Austria, Belgium, Denmark, Great Britain and France has been established to examine the mechanisms of deterioration. The experimental techniques used in the analyses are X-ray fiber diffraction, electron paramagnetic resonance spectroscopy, hydrothermal stability measurements and amino acid determination.

Department of Chemistry
High Temperature Corrosion

A large number of important engineering systems operating at high temperatures (480-1100°C) involve contact of metallic or ceramic materials with combustion product gases or other oxidizing gases containing inorganic impurities, e.g. gas turbines, steam generators, incinerators, petrochemical process vessels. As the gases are cooled, fused salt films may condense on the hardware to generate highly corrosive conditions analogous in some aspects to aqueous atmospheric corrosion. Some other engineering systems, such as the molten carbonate fuel cell, heat treatment baths, high-temperature homogeneous catalysis etc. use molten salts to accelerate the electrochemical and chemical reactions. When materials come into contact with corrosive molten salt films one can also expect high rates of the corrosion reactions but in this case the acceleration is undesirable and makes corrosion more severe than in aqueous solutions. However the availability of high quality fossil fuels becomes limited, and technologies of solid waste utilization and other efficient energy conversion processes are under development. The damage of hot corrosion is likely to increase. The most important features of hot corrosion are: 1. Generally molten salts are ionic conductors so that the corrosion attack must be electrochemical in nature. 2. Oxyanion molten salts (silicates, sulphates, carbonates, phosphates etc.) exhibit an acid-base behavior. Acidity of the electrolyte often defines the mechanism of the corrosion process. 3. The main products of the reaction between metal and molten salt layer are oxides. Solubility of these oxides in the melt defines the corrosion resistance.

Alcohols and diols in aqueous solution

Experimental measurements of various properties of water, small alcohols and diols are coupled with ab initio studies and with model calculations in an attempt to gain better description of hydrogen bonding. Experiments include 17-O NMR (at the University of Bonn), infrared spectrometry, viscosity.
Development of new methods for asymmetric synthesis
The overall goal of this project is to develop new and efficient methods for stereoselective asymmetric organic synthesis, i.e. the synthesis of organic compounds in a single three-dimensional form. A focus of our research in this area in recent years has been the study of asymmetric Wittig-type reactions. In future work, our work will be expanded to cover several other powerful reaction types as well. The research involves both experimental synthetic work and computational modelling.
Financing sources
Source: Internal funding (public)
Name of research programme: DTU-Su Stipendium, Eksperiment
Project: PhD

Synthesis of natural products and their analogs
Our work within this project is aimed at the synthesis of compounds (either natural products or their analogs) possessing interesting and potentially useful biological activity. An important aspect is to use synthetic methods developed within our group as key steps in the synthetic plan. Furthermore, the compounds synthesized will be tested for biological activity and mode of action, in collaboration with other researchers who are experts in these areas. Among targets currently under investigation are several macrolides and alkaloids with antitumor and/or antibiotic properties.

Department of Organic Chemistry
Department of Chemistry
Royal Danish School of Pharmacy
University of Tartu
Period: 01/09/1996 → 31/12/2000
Number of participants: 8
Project participant:
Lundt, Inge (Intern)
Tanner, David Ackland (Intern)
Pedersen, Torben Møller (Intern)
Helquist, Paul (Intern)
Norrby, Per-Ola (Ekstern)
Tullis, Joshua (Ekstern)
Vares, Lauri (Ekstern)
Project Manager, organisational:
Rein, Tobias (Intern)

Kinetics and Electronic Spectral Patterns.
Department of Chemistry
Period: 01/08/1996 → 28/09/2001
Number of participants: 5
Phd Student:
Andersen, Niels Højmark (Intern)
Main Supervisor:
Ulstrup, Jens (Intern)
Examiner:
Søtofte, Inger (Intern)
Larsen, Leif Erik (Ekstern)
Nielsen, Hans Toftlund (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsstip.-SU, Eksp
Project: PhD

Natural products synthesis and combinatorial chemistry
Department of Chemistry
Period: 01/08/1996 → 31/05/1998
Number of participants: 2
Phd Student:
Hansen, Stefan Philip (Intern)
Main Supervisor:
Nielsen, John (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: DTU-Su Stipendium, Eksperiment
Project: PhD

**Scanning Probe undersøgelser af adsorberede**
Department of Chemistry
Period: 01/08/1996 → 23/11/1999
Number of participants: 4
Phd Student:
Friis, Esben P. (Intern)
Main Supervisor:
Ulstrup, Jens (Intern)
Examiner:
Bagger, Sven (Intern)
Grey, Francois (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: DTU-Su Stipendium, Eksperiment
Project: PhD

**Spektroskopiske studier af lipidmembraner**
Department of Chemistry
Period: 01/07/1996 → 14/09/1999
Number of participants: 4
Phd Student:
Trandum, Christa (Intern)
Supervisor:
Jørgensen, Kent (Intern)
Westh, Peter (Intern)
Main Supervisor:
Mouritsen, Ole G. (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: DTU-Su Stipendium, Eksperiment
Project: PhD

**Kombinatorisk og Bioorganisk Kemi**
Department of Chemistry
Period: 01/06/1996 → 17/05/2000
Number of participants: 3
Phd Student:
Lyngsø, Lars Ole (Intern)
Main Supervisor:
Nielsen, John (Intern)
Examiner:
Tanner, David Ackland (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Forskningsrådsstip.-SU, Eksp
Project: PhD
Kombinatorisk Kemi
Department of Chemistry
Period: 01/02/1996 → 18/10/2000
Number of participants: 4
Phd Student:
Carstensen, Elisabeth Vang (Intern)
Main Supervisor:
Nielsen, John (Intern)
Examiner:
Madsen, Robert (Intern)
Pedersen, Erik Bjerregaard (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-Su Stipendium, Eksperiment
Project: PhD

Materialeegenskaber af højtemperatur superledere
Department of Chemistry
Period: 01/02/1996 → 20/05/1999
Number of participants: 4
Phd Student:
Frello, Thomas (Intern)
Supervisor:
Engell, John Emil (Intern)
Main Supervisor:
Høj, Jakob Weiland (Intern)
Examiner:
Freltoft, Torsten (Ekstern)

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

Structural and electrical properties of perovskites
The purpose of the project is to investigate possible correlations between ionic conductivity and crystal structure of metal oxides with the perovskite structure. The perovskite group of materials possess a wide range of compositional and structural modifications with interesting properties, e.g. ionic conductivity, superconductivity and reactivity as sensors and catalysts.

Department of Chemistry
Risø National Laboratory for Sustainable Energy
Period: 01/02/1996 → 31/03/2000
Number of participants: 4
Project participant:
Larsen, Dorthe (Intern)
Mogensen, Mogens (Intern)
Poulsen, Finn Willy (Intern)

Project Manager, organisational:
Nielsen, Kurt (Intern)

Strukturelle og elektriske egenskaber af perovskitter
Department of Chemistry
Period: 01/02/1996 → 24/07/2000
Number of participants: 3
Phd Student:
1,5-Anhydro-D-Fructose: Structure, Chemical Behaviour, Derivatisation

Starch can be enzymatically degraded to give 1,5-anhydro-D-fructose (AF), a compound which can only be obtained in small amounts by chemical methods. The exact structure has, however, been discussed for years, and until now not determined. Investigation of the chemical reactions together with preparation of derivatives should give a better understanding of the structure of AF. Furthermore the use of AF as a chiral synthon should be investigated. The preparation of C-6 acylated derivatives of AF with fatty acids should be undertaken, both chemically and by enzymatic methods. These products should be investigated as emulgators.
Lundt, Inge (Intern)
Examiner:
Pedersen, Christian (Ekstern)

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

Calculation of the Electronic Structures of Molecules
Detailed calculations of molecular electronic structures with emphasis on bonding, spin-density, catalytic activity, geometry, and spectroscopic properties. Targets for the investigations are small organic and inorganic molecules as well as transition metal complexes. Recent studies include (S3)-, (VO2SO4)-, (Cu(H2O)6)2+, and the interaction between ammonia and sulfur dioxide. In the last case, there is a special emphasis on the low lying triplet states. The calculations apply SCF, MCSCF, CI and perturbation methods using the program systems Gaussian-94 and MOLCAS-3 as well as locally developed programs. The project is partly financed by a grant from The Danish Natural Sciences Research Council (SNF).

Department of Chemistry
Period: 01/01/1996 → 31/12/1997
Number of participants: 1
Project Manager, organisational:
Johansen, Helge (Intern)

Chemical Reaction Dynamics
Elementary chemical reactions are studied on an atomic level with molecular reaction dynamics simulations. If quantum effects are important they are included by propagating the relevant degrees of freedom using the time dependent Schrödinger equation. In particular, the dissociation of simple molecules like N2 on catalytic metal surfaces has been studied. This is the "bottleneck" in many chemical reactions involving N2 and the simulations have given a detailed insight in the dissociation process otherwise impossible to obtain. Another type of reactions studied is the laser induced dissociation of molecules, where the idea is to control the chemical reaction by a proper design of the laser pulse. In particular, the effect of the presence of a condensed phase on the excitation and reaction is studied by enclosing the molecules in a small cluster of inert molecules or in the bulk of a an inert crystal or fluid.

Department of Chemistry
Period: 01/01/1996 → …
Number of participants: 2
Project participant:
Henriksen, Niels Engholm (Intern)
Project Manager, organisational:
Hansen, Flemming Yssing (Intern)

Combinatorial and Bioorganic Synthesis
The project "Combinatorial and Bioorganic Synthesis" is a collaborative project between the combinatorial and solid-phase synthesis group at the DTU and Dr. Mikael Bols group at Aarhus University. The project is financed by the Danish Research Council. The project focus is on the application of combinatorial chemical techniques for approaching or solving scientific problems of chemical, medicinal or biological relevance. The specific projects embrace a) "Glycobiotics" which includes synthesis of oligosaccharide mimetic and construction of combinatorial libraries of glycobiotics. b) "Approaching natural product synthesis by combinatorial chemistry" which include convergent synthesis of Actinomycin D analogues, the implementation of double-combinatorial chemistry, and combinatorial synthesis of balanol analogues.

Department of Organic Chemistry
Aarhus University
Period: 01/01/1996 → 31/12/1998
Number of participants: 6
Project participant:
Complex formation in melts and in relation to solid state chemistry

The dependence of Raman and IR spectra on the structures of the scattering molecular fragments is studied. Many substances react in ways not totally known. The elucidation of the reactions and the structures of the new complexes is the aim of this project. The determination of solid state structures by means of the Rietveld profile refinement of X-ray diffraction data for powder samples is an important aspect of the project.

Department of Chemistry

Crystal structure determinations of two synthetic phases

Experimental studies of the phase systems Cu-Te-Sb and Cu-Te-S at temperatures between 350 and 1000 °C have shown the existence of some not previously described Cu-rich phases. One phase, phase A, is stable at temperatures between 400 and 900 °C. At 700 °C it shows maximum variation in chemical composition from Cu69Te8Sb23 to Cu63Te52Sb5. The other phase, phase B, is stable at temperatures between 350 and 675 °C. It displays maximum variation in chemical composition at 675 °C from 62Te20S18 to Te34S4. Presently crystal structure investigations is carried out on the two phases. This research takes place in cooperation with associate professor I. Søtofte at IK, DTU and professor E. Makovicky at The Geological Institute, KU.

Department of Geology and Geotechnical Engineering

Determination of two-dimensional saturation profiles in cores by nuclear techniques

Department of Automation

Department of Physics

Department of Chemistry
Department of Chemical and Biochemical Engineering

Geological Survey of Denmark and Greenland
Period: 01/01/1996 → 31/12/1996
Number of participants: 3
Project participant:
Korsbech, Uffe C C (Intern)
Ølgaard, Povl Lebeck (Intern)
Project Manager, organisational:
Sletsgaard, Jan (Intern)

Financing sources
Source: Unknown
Name of research programme: Ukendt
Amount: 189,000.00 Danish Kroner

Electrochemical and Spectroscopic Investigation of Electrochemical Cells and Catalysts
The project is concerned with a study of the different non-aqueous chemical processes using electrochemical (cyclic voltammetry, square-wave voltammetry, chronoamperometry etc.) and spectroscopic (Raman, IR, ESR, NMR etc.) techniques. All the studied processes involve electrochemical steps or electrochemical techniques were used for their study. The project involves investigation of following electrochemical reaction or systems: 1. Electroplating with refractory metals (niobium, tantalum) from molten salts. 2. Phosphoric acid, molten carbonate and solid oxide fuel cells. 3. Development of the active materials for nickel- metal hydride batteries. 4. Study of the mechanism of the catalytic SO2 oxidation using electrochemical techniques.

Department of Chemistry

Electrokinetics in oil recovery
Investigations of electrokinetics in reservoir chalk. Estimation of the the use of electrokinetics in secondary oil recovery.

Department of Chemistry

Electrokinetics in oil recovery
Investigations of electrokinetics in reservoir chalk. Estimation of the the use of electrokinetics in secondary oil recovery.

Department of Chemistry

Department of Chemistry

Electrokinetics in oil recovery
Investigations of electrokinetics in reservoir chalk. Estimation of the the use of electrokinetics in secondary oil recovery.

Department of Chemistry
In-vivo clearance of man made vitreous fibres
Physico-chemical and statistical analysis of the results of clearing of man made vitreous fibres in rat lungs.

Iridoider i Loasaceae og deres biosyntese

Laser control of chemical reactions
The course of chemical reactions is determined by the time-dependent Schrödinger equation. The outcome of reactions can be changed by applying external fields such that the formation of unwanted products can be avoided or minimized. Current projects include: 1) Laser control of bond-selective fragmentation 2) Laser control of electronic motion

Micro-Raman-spectroscopy
Micro-Raman-spectroscopy is a universal analytical technique based on light scattering under a confocal microscope. It is used for the identification of molecules in gasses, liquids and solids. With our instrument analyses can be made from small samples, provided that they do not fluoresce under the influence of the laser illumination. Raman micrographs with a 1 micrometer resolution can be obtained.
Molecular reaction dynamics
At the fundamental level the course of chemical reactions is determined by the time-dependent Schrödinger equation. Current projects include: 1) Wave packet dynamics of nuclear motion. 2) Non-adiabatic dynamics in molecules. 3) Reaction dynamics - simple models of laser-induced dissociation dynamics. 4) Femtosecond chemistry, real-time detection of chemical reactions.

Opbygning af ladingsevne normal til vand
Physisorption of Molecules to Solid Surfaces
A great variety of molecules, from a simple molecule like N2 to long alkane molecules like c32H66, has been studied by molecule dynamics methods when they are adsorbed on a solid surface. Of particular interest has been the microscopic mechanism of melting and rotational disorder transitions. The interaction models used in the simulations have also been checked and in some cases improved as a result of our studies. Dynamic processes like diffusion and dynamical excitations in the films have been studied in great detail and lately the effect of a dynamic substrate on the excitations in the films have been evaluated. A particular focus in the long alkane film studies is the selective adsorption of a single chemical species from a multicomponent fluid mixture of importance for coatings, lubricants and adhesives. The goal is to provide a microscopic knowledge of these systems as a complement to the macroscopic thermodynamical understanding and to study the kinetics and dynamics of polymer mixtures at an atomic level. An important element in the theoretical studies is that they usually are conducted in close collaboration with foreign groups who conduct experimental studies of the systems studied theoretically. This is of great importance for the understanding of the experimental data and the theoretical results and at the same time of great mutual inspiration. Scientific visitors in 1998: H. Taub and L.W. Bruch

Raman & IR Research on SOFC Materials
Attempts to characterize spectroscopically the materials used for state of the art high temperature Solid State Fuel Cells (SOFCs). SOFCs are of use for converting fuels like methane and hydrogen to electric power efficiently.

Department of Chemistry
Norwegian University of Science and Technology
Period: 01/01/1996 → 31/12/2002
Number of participants: 5
Project participant:
Kjerulf-Jensen, Ninette (Intern)
Poulsen, Finn Willy (Intern)
Glerup, Marianne (Intern)
Developement of Methods for the Enantioselective Synthesis of Chiral Carbo- and Heterocycles.

Department of Chemistry
Period: 01/10/1995 → 16/12/1998
Number of participants: 3
Phd Student: Fensholdt, Jef (Intern)
Main Supervisor: Tanner, David Ackland (Intern)
Examiner: Pedersen, Erik Bjerregaard (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsstip.-SU, Eksp
Project: PhD

Rheology of Grafted Chains under Shear
Non-equilibrium molecular dynamics simulations are applied to investigate the effect of coating two opposite walls with amphiphilic molecules on the fluid structure, friction and viscosity of a pure solvent. This is a typical industrial problem encountered in fabric softening, where amphiphiles (surfactants) are added during the washing to enhance the condition of the fabric and the conditioning of hair before wet combing. In particular, we like to address the following fundamental questions: (1) How does grafted charged amphiphiles will change the viscosity profile? (2) Is the stress (friction) profile constant across the shear field? (3) How does the solvent will adapt to the cahrged amphiphiles? (4) Are solvent molecules trapped in the organic layer? (5) How does flexibilty of the chains influence the rheological properties?

Department of Chemistry
Department of Chemistry
Period: 01/10/1995 → …
Number of participants: 1
Project Manager, organisational:
Peters, Günther H.J. (Intern)

**Stereoselektiv totalsyntese**

Department of Chemistry
Period: 01/10/1995 → 09/12/1998
Number of participants: 4
Phd Student:
Kornø, Hanne Tøfting (Intern)
Main Supervisor:
Tanner, David Ackland (Intern)
Examiner:
Begtrup, Mikael (Ekstern)
Kjær, Anders (Intern)

**Financing sources**
Source: Internal funding (public)
Name of research programme: Forskningsrådsstip.-SU, Eksp
Project: PhD

The structure and properties of zeolites.
Zeolitic materials consist of three-dimensional alumino-silicate frameworks, surrounding cavities and channels. These materials may be regarded as molecular test tubes: Through variations in the framework, and in the cavities and channels, the materials will be selective to different ions and molecules, and thereby achieve widely different properties. Zeolitic materials are used in huge quantities as for example catalysts in petro-chemical industry, water softener in washing powder, and absorbants in different types of filters. The crystal structures of natural and synthetic zeolites are studies mainly by means of powder diffraction, using neutrons, and X-rays, and the structures are related to the physical and chemical properties. Using synchrotron radiation, the dynamics of the zeolites during dehydration processes are studied in situ.

Department of Chemistry
Department of Chemistry
University of Milan
Brookhaven National Laboratory

Norwegian University of Science and Technology
Period: 01/09/1995 → …
Number of participants: 4
Project participant:
Artioli, Gilberto (Ekstern)
Hanson, Jonathan (Ekstern)
Nicholsen, David (Ekstern)

Ståhl, Kenny (Intern)
Project Manager, organisational:

**Tungmetallers bindingsforhold i jord**

Department of Chemistry
Period: 01/09/1995 → 29/03/2001
Number of participants: 4
Phd Student:
Karlsmose, Bodil (Intern)
Supervisor:
Villumsen, Arne (Intern)
Main Supervisor:
Bech-Nielsen, Gregers (Intern)
Examiner:
Skou, Eivind Morten (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Blandet Finansiering-SU
Project: PhD

Udvikling af højtemperatur superledere
Department of Chemistry
Department of Geology and Geotechnical Engineering
Materials Research Division
Haldor Topsoe AS
Number of participants: 4
Project participant:
Christiansen, Jens Kristian S. (Intern)
Tidemand-Petersson, Camilla (Intern)
Diaz, Hektor Osvaldo Ampuero (Intern)
Project Manager, organisational:
Høj, Jakob Weiland (Intern)

Financing sources
Source: Unknown
Name of research programme: Uendt
Amount: 3,000,000.00 Danish Kroner
Project

Elektrode kinetik i højtemperatur brændselceller
Department of Chemistry
Period: 01/08/1995 → 01/01/1999
Number of participants: 4
Phd Student:
Bay, Lasse (Intern)
Main Supervisor:
Jacobsen, Torben (Intern)
Examiner:
Skaarup, Steen (Intern)
Skou, Eivind Morten (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-Su Stipendium, Eksperiment
Project: PhD

Iridoidglucosider som substrater ved syntese af biologisk aktive
Department of Chemistry
Number of participants: 5
Phd Student:
Rasmussen, Jon Holbech (Intern)
Supervisor:
Franzyk, Henrik (Intern)
Main Supervisor:
Jensen, Søren Rosendal (Intern)
Examiner:
Tanner, David Ackland (Intern)
Wengel, Jesper (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-Su Stipendium, Eksperiment
Project: PhD

Iridoidglucosider som substrater ved syntese af biologisk aktive cyclopentanderivater

Department of Chemistry
Period: 01/08/1995 → 15/06/1999
Number of participants: 5
Phd Student:
Frederiksen, Signe Maria (Intern)
Supervisor:
Franzyk, Henrik (Intern)
Main Supervisor:
Jensen, Søren Rosendal (Intern)
Examiner:
Begtrup, Mikael (Ekstern)
Damtoft, Søren (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsstip.-SU, Eksp
Project: PhD

Karakterisering af smeltebade til pletteringsprocesser

Department of Chemistry
Number of participants: 3
Phd Student:
Gillesberg, Bo (Intern)
Main Supervisor:
Bjerrum, Niels J. (Intern)
Examiner:
Larsen, Leif Erik (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-Su Stipendium, Eksperiment
Project: PhD

Fine chemicals and drugs from plants.
Compounds isolated from plants can often be isolated in notable amounts and may then be interesting as synths for pharmacologically interesting compounds. Antirrhinoside and catalpol are such compounds; they are the main constituents in snapdragon (Antirrhinum major) and scullcap (Scutellaria albida), respectively. These plants can be grown as alternative crops on fields laid bracken. The advantage when using such compounds as starting materials in synthesis is the inherent stereochemical integrity which controls the stereochemistry in the further synthetic steps leading to biologically active compounds such as analogues of prostaglandines, jasmonic acid as well as carbocyclic nucleosides.

Department of Organic Chemistry
Department of Chemistry
Royal Danish School of Pharmacy
Statens Planteavlsløsning
Period: 01/07/1995 → 30/06/2000
Number of participants: 7
Alkylgrupper kemi i tris (pyrazolyl) borat konplexer af tidlige overgangsmetaller og lantanider

Department of Chemistry
Period: 01/05/1995 → 23/09/1998
Number of participants: 4
Phd Student:
Mikkelsen, Gitte Kobberøe (Intern)
Supervisor:
Lundt, Inge (Intern)
Main Supervisor:
Tanner, David Ackland (Intern)
Examiner:
Begtrup, Mikael (Ekstern)

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

Højtemperatur korrosion under industrielle

Department of Chemistry
Period: 01/05/1995 → 05/02/2002
Number of participants: 6
Phd Student:
Cappeln, Frederik Vilhelm (Intern)
Supervisor:
Petrushina, Irina (Intern)
Main Supervisor:
Bjerrum, Niels J. (Intern)
Examiner:
Skou, Eivind Morten (Ekstern)
Bech-Nielsen, Gregers (Intern)
Karlsson, Asger (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Blandet Finansiering-SU
Project: PhD

Stabilization of Landslides in Slovakia
Electroosmotic dewatering of fine grained material is used for the stabilization of sliding areas

Department of Geology and Geotechnical Engineering
In situ STM

In situ Scanning Tunnelling Microscopy (in situ STM). Imaging of electrochemistry on surfaces in electrolytes in real time. Imaging of metal electrocrystallisation from the initial stages to the level of bulk growth. Imaging of immobilised proteins and enzymes at the molecular level and investigations of the electrochemistry in real time. Analytically, the number of immobilised enzyme molecules as determined by imaging is related to the enzymatic activity.

Department of Chemistry

Period: 01/04/1995 → 01/10/1997
Number of participants: 4
Project participant:
Bucka-Christensen, Thomas (Intern)
Laursen, Søren (Intern)
Kisling, Leif (Ekstern)

Project Manager, organisational:
Villumsen, Arne (Intern)

Financing sources
Source: Unknown
Name of research programme: Ukendt
Amount: 1,000,000.00 Danish Kroner

Department of Chemistry

Partikelinteraktion og væksfænomener: Et AFM-studie af sol-gel processer

Department of Chemistry
Period: 01/03/1995 → 04/12/1998
Number of participants: 3
Phd Student:
Pedersen, Henrik Guldberg (Intern)
Supervisor:
Engell, John Emil (Intern)
Main Supervisor:
Høj, Jakob Weiland (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-Su Stipendium, Eksperiment
Project: PhD

Department of Chemistry

Femtokeri

Number of participants: 4
Phd Student:
Grønager, Michael (Intern)
Supervisor:
Henriksen, Niels Engholm (Intern)
Main Supervisor:
Dahl, Jens Peder (Intern)
Examiner:
Hansen, Flemming Yssing (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-Su Stipendium, Eksperiment
Project: PhD

Membranaktive molekylers vekselvirkning med lipidmembraner
Department of Chemistry
Period: 01/02/1995 → 02/06/1998
Number of participants: 5
Phd Student:
Sabra, Mads Christian (Intern)
Supervisor:
Jørgensen, Kent (Intern)
Main Supervisor:
Mouritsen, Ole G. (Intern)
Examiner:
Hvidt, Søren (Ekstern)
Rasmussen, Kjeld (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-Su Stipendium, Eksperiment
Project: PhD

Chemical Vapor Deposition (CVD)
The primary objective of the CVD-research is tantalum coating of stainless steel, carbon steel, nickel, copper, titanium and aluminum by CVD. Tantalum is deposited from TaCl5 by reduction with hydrogen at 625-1000 C. The TaCl5 is generated directly from Ta and Cl2 at 400-600 C prior to mixing with H2 and heating to the deposition temperature. Niobium and tungsten coatings are deposited by similar processes. Catalytically active platinum layers has been prepared by metalorganic-CVD. Platinum is deposited from platinum bis penta-2,4-dion in hydrogen at 300 C and 0,1 mbar. Copper deposition on nickelbased alloys from copper bis 1,1,1,5,5,5-hexafluoropenta-2,4-dion is a new CVD activity and subject of a PMP (3 students).

Department of Chemistry
Department of Chemistry
Period: 01/01/1995 → …
Number of participants: 3
Project participant:
Eriksen, Søren (Intern)
Christensen, Erik (Intern)
Project Manager, organisational:
Bjerrum, Niels J. (Intern)
Project

Conversion of Methane
The purpose of this project is to develop a direct conversion process to convert methane (from natural gas) to, for example, methanol which can easily be transported and which is also a more flexible and valuable raw chemical. The project aims at developing a process which is selective and effective enough so that as little methane as possible will be re-circulated in the process. Several types of catalysts have been found in connection to the project, and very high methanol yields have been achieved by using them.

Department of Chemistry
Department of Chemistry
Period: 01/01/1995 → 31/12/2002
Number of participants: 3
Iminosugars/Azasugars - Glycosidase Inhibitors

Glycosidases and glycosyltransferases are instrumental in the processing of various glycosylated proteins, which are ubiquitous in nearly all forms of life and play an important role in molecular recognition, adhesion and transport. The profound impact of these enzymes on life processes has made them desirable targets for inhibition. Glycophosphorylating inhibitors have been used to treat diabetes, and have a potential as antiviral and antitumor agents. Important groups of inhibitors are azasugars and carbasugars, compounds which have structure similar to sugars, but in which the ring oxygen has been replaced by a nitrogen or a methylene group, respectively. These compounds mimic the sugar in question by occupying the catalytically active site in the enzyme, thus preventing the hydrolysis/glycosylation. Recently we found that azasugars having the anomeric carbon replaced by a nitrogen were very potent beta-glycosidase inhibitors. Our approach to synthesize azasugars is stereocontrolled reactions starting from the chiral pool, namely the easily available sugar lactones. We have developed one step procedures for regioselective functionalizations of aldolactones from which azasugars can be prepared in two to four steps. This appears to be the most general non-enzymatic synthetic procedure of potentially glycosidase inhibitors from carbohydrate precursors without the use of any protecting groups. The investigations will focus on synthesis of aza/iminoses having nitrogen in place of the ring oxygen, as well as nitrogen replacing the anomeric carbon, having other hydroxyl groups modified as well in search for good glycosidase inhibitors/transition state analogues. More specific studies towards synthesis of inhibitors for a polysaccharide degrading enzyme is in progress.

Department of Organic Chemistry
Graz University of Technology
Period: 01/01/1995 → 01/01/9999
Number of participants: 7
Project participant:
Godskesen, Michael Anders (Intern)
Malle, Birgitte Mølholm (Intern)
Tagmose, Tina Møller (Intern)
Andersen, Søren Møller (Intern)
Wagner, Sussi Holstein (Intern)
Stütz, Arnold E. (Ekstern)
Project Manager, organisational:
Lundt, Inge (Intern)

Financing sources
Source: Unknown
Name of research programme: Ukendt
Amount: 1,100,000.00 Danish Kroner

Macrocyclic Organic Molecules

A large number of various macrocyclic organic molecules have been prepared by prof. Jan Becher and his group at Odense University. In most cases they tend to form crystals of rather low quality. However, in several cases suitable crystals for X-ray crystal structure determination have been obtained. The structures are in many cases quite big. Therefore, data collection and structure determination has been greatly facilitated by the recent acquisition of a diffractometer with a CCD area detector. The molecules often contain tetrafluorovanadamene(TTF) building units. In some cases the molecules form catenanes, i.e. mechanically interlocked molecular systems, and some times cages are formed with included guest molecules.

Department of Chemistry
University of Southern Denmark
Period: 01/01/1995 → ...
Number of participants: 2
Project participant:
Becher, Jan (Ekstern)
Polymer Electrolyte Fuel Cell
The group's research in this area is focused on the investigation and development of low platinum loading gas diffusion electrodes (GDE) for the polymer electrolyte fuel cell (PEFC). Tests are being conducted on a single fixed test cell. Power densities of more than 0.5 W/cm² are achieved when running the cell on pure hydrogen and oxygen at 80°C and ambient pressure. Operational parameters such as gas humidification, pressure, temperature and composition of fuel and oxidant gases are also investigated.

Department of Chemistry

Spontan dannelse af uorden i glasser

Styring af de stereokemiske forløb ved reduktioner med bagegær
Syntese af chirale molekyler med potentiel glycosidaseinhibitor-effekt

Department of Chemistry
Period: 01/01/1995 → 16/01/1999
Number of participants: 3
Phd Student:
Godskesen, Michael Anders (Intern)
Main Supervisor:
Lundt, Inge (Intern)
Examiner:
Begtrup, Mikael (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsstip.-SU, Eksp
Project: PhD

The hydrolysis of phosphate esters by dinuclear transition metal complexes

Department of Chemistry
Period: 01/12/1994 → 29/06/1998
Number of participants: 5
Phd Student:
Ghiladi, Morten (Intern)
Main Supervisor:
Ulstrup, Jens (Intern)
Examiner:
Bagger, Sven (Intern)
Brorsen, Michael Christian (Ekstern)
Nielsen, Hans Toftlund (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsstip.-SU, Eksp
Project: PhD

Fluoride in Magadi Salts
High Fluoride intakes via water is common in dry or volcanic regions in Africa. This calamity is aggravated with the use of Magadi (sodium hydrogen carbonate) with high Fluoride concentrations. The Ph.D. project covers the occurrence of contaminated Magadi, the crystallization processes in the alkaline lakes, and the technical possibilities for purifying Magadi for human consumption.

Department of Environmental Science and Engineering
Department of Chemistry
Department of Chemistry
Felix Mtalo
Elian Dahi
Period: 01/09/1994 → 31/10/1997
Number of participants: 3
Project participant:
Nielsen, Joan Maj (Intern)
Engell, John Emil (Intern)
Project Manager, organisational:
Tjell, Jens Christian (Intern)

Financing sources
Source: Unknown
Name of research programme: U bundt
Amount: 1,000,000.00 Danish Kroner
Project
Multilayer Actuators: Metal-Ceramic Compatibility as a Function of Composition, Sintering Temperature and Use

Department of Chemistry
Period: 01/08/1994 → 12/03/1999
Number of participants: 3
Phd Student: Ringgaard, Erling (Intern)
Main Supervisor: Høj, Jakob Weiland (Intern)
Examiner: Hansen, Flemming Yssing (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-Su Stipendium, Eksperiment
Project: PhD

Udvikling af smøremidler til koldflydeprocesser i rustfast stål

Department of Chemistry
Period: 01/04/1994 → 01/04/1997
Number of participants: 3
Phd Student: Steenberg, Thomas (Intern)
Main Supervisor: Bjerrum, Niels J. (Intern)
Examiner: Danckert, Joachim (Ekstern)

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

Implementation and automation of trace organic analysis in mobile laboratories

Department of Chemistry
Period: 01/02/1994 → 22/07/1997
Number of participants: 5
Phd Student: Nilsson, Torben (Intern)
Main Supervisor: Madsen, Jørgen Øgaard (Intern)
Examiner: Grøn, Christian (Intern)
Hansen, Elo Harald (Intern)
Svensmark, Bo (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Anden Ef-Finansiering-SU
Project: PhD

Metalloproteiners Dynamik, Metalsubstitution og Totalsyntese

Department of Chemistry
Period: 01/02/1994 → 30/04/1997
Number of participants: 4
Phd Student: Pedersen, Marianne Vind (Intern)
Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsstip.-SU, Eksp
Project: PhD

Molekylære Vekselvirkninger i Lipidmembraner studeret ved kalorimetri og fluorescensspektroskop!

Department of Chemistry
Period: 01/02/1994 → 23/07/1997
Number of participants: 5
Phd Student:
Risbo, Jens (Intern)
Supervisor:
Jørgensen, Kent (Intern)
Main Supervisor:
Mouritsen, Ole G. (Intern)
Examiner:
Hansen, Flemming Yssing (Intern)
Præstegaard, Eigil (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsstip.-SU, Eksp
Project: PhD

Semi-klassiske metoder i molekylær dynamik

Department of Chemistry
Period: 01/02/1994 → 30/04/1997
Number of participants: 5
Phd Student:
Møller, Klaus Braagaard (Intern)
Supervisor:
Henriksen, Niels Engholm (Intern)
Main Supervisor:
Dahl, Jens Peder (Intern)
Examiner:
Child, Mark S. (Ekstern)
Hansen, Flemming Yssing (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-Su Stipendium, Eksperiment
Project: PhD

Electronic Processes in Nanoscale Systems

The aim of this new untraditional research is to disclose and map structure and electronic function of individual molecules and biological macromolecules at single-molecule level. The research rests on: Theory of Molecular Electron and proton Transport in Chemical and Biological Systems. State-of-the-art electrochemistry, and In Situ and Electrochemical Scanning Tunneling and Atomic Force Microscopy of Biological Macromolecules

Department of Chemistry
Period: 01/01/1994 → ...
Number of participants: 12
Project participant:
Lubricants for Cold Forging of Stainless Steel

One of the major problems related to cold forging of stainless steel is to secure sufficient lubrication during the process. The severe conditions during the process (i.e. high normal pressures and large surface expansion) usually requires a two component lubricant system consisting of a porous carrier coating lubricated with a suitable lubricant. This project deals with the development of two new lubricant systems for cold forging of stainless steel. The lubricant systems are based on zinc phosphate and iron(III) chloride respectively. The zinc phosphate coating serves as a porous “carrier coating” for the actual lubricant (i.e. sodium stearate or MoS2). Iron(III) chloride can be used alone or in combination with MoS2 or graphite. The work has been focusing on application methods, characterisation and tribological tests. An electrochemical method for depositing zinc/calcium phosphate coatings on stainless steel from an aqueous nitric acid solution has been developed. The method involves hydrogen evolution at the surface of the specimen and the deposition occurs due to decreasing solubility of the metal phosphates at increasing pH. The lubrication mechanism of iron(III) chloride is believed to involve the reaction between iron(III) chloride and the stainless steel surface to form iron(II) chloride. Results from backward can extrusion tests confirm that this reaction contributes significantly to the lubrication properties. Backward can extrusion tests of zinc/calcium phosphate (lubricated with sodium stearate) and iron(III) chloride show that a height/diameter ratio of more than two can be obtained. A height/diameter ration of 1.2 can be obtained with the current State of The Art lubricant system (Iron oxalate combined with MoS2).

Department of Chemistry

Partikel interaktion i kolloidale systemer

Department of Chemistry

Phosphoric Acid Fuel Cells (PAFC)

The research activity in this area is mainly concentrated on the technology of the PAFC stack. Manufacturing of Gas diffusion electrodes and related techniques are further improved in order to enhance the catalytic efficiency for oxygen
reduction. Chemical and electrochemical techniques are also under development for minimizing the poisoning effect of fuel impurities on the anodic catalysts.

Properties and Applications of Electronic Molecular Phase-Space Functions
A very intuitive representation of quantum-mechanical state vectors is obtained when one works in phase space and introduces the Wigner distribution function, which has the position and momentum densities as proper marginals. In the past, we have evaluated and analyzed the electronic Wigner functions for a number of atoms and small molecules. By averaging a Wigner function with the dynamical phase-space functions corresponding to the kinetic energy or the two-particle exchange energy over the momentum variables, one may obtain well-defined densities in position space for these quantities, so-called local densities, as we showed several years ago. We are now extending our work on Wigner functions and local densities in order to evaluate their use in many-electron density functional theories which today form the basis for much work on electronic structures. The project is partly financed by a grant from The Danish Natural Sciences Research Council (SNF).

Thermochemistry in Molten Salts
The main purpose of this project is to obtain relevant thermochemical information on molten salt systems - especially those which are of importance in other projects dealt with in the Materials Science Group at Department of Chemistry. Most of the work is carried out in a high temperature heat-flux-calorimeter (max. 550 °C) constructed at AMT and in our workshops. Currently molten salt mixtures containing aluminium and alkali halogenides are investigated in the temperature range 200 to 350 °C.
Biological Sequence Analysis
The Center for Biological Sequence Analysis conducts basic research in bioinformatics - a rapidly growing area in the field of molecular biology. The overall goal of the research is to obtain knowledge of the complex relations between sequence composition - the content and order of the chemical building blocks - and macromolecular structure and function. In addition, the research is aimed at creating entirely new possibilities in the study of evolutionary processes by comparison of sequence patterns across species. The tremendous growth in the amount of sequence and structure data has brought about a radical change in the possibilities of developing powerful computer methods for classification, prediction and comparison of molecular structure and function. The work of the center is especially focussed on novel data driven computational methods, such as artificial neural networks and hidden Markov models.

Financing sources
Source: Unknown
Name of research programme: 
Amount: 25,000,000.00 Danish Kroner
Source: Unknown
Name of research programme: 
Amount: 250,000.00 Danish Kroner
Source: Unknown
Name of research programme: 
Amount: 325,000.00 Danish Kroner
Source: Unknown
Name of research programme: 
Amount: 860,000.00 Danish Kroner
**Electrochemistry in Molten Salts**

A noticeable part of the important electrochemical processes proceeds at high temperatures using molten salt electrolytes. Electrochemistry of molten salts started at the beginning of the nineteenth century, when H. Davy extracted potassium and sodium from molten hydroxides by electrolysis in 1807. At the end of the nineteenth century C. M. Hall and P. L. T. Héroult invented the electrolytic route to aluminium production, and this led to the establishment of the largest industry of metal extraction from molten salts. Compared to aqueous solutions and organic electrolytes, the advantages of molten salts are the following: 1. The electrical conductivity is higher, i.e. about an order of magnitude higher than that of aqueous solutions and several orders higher than that of organic electrolytes. 2. The electrode reactions are faster at high temperatures. 3. The absence of water in the molten salt and therefore no hydrogen reduction. As a result metals with more negative potentials than hydrogen can be reduced. Electrolytic production of metals from molten salts, with the Hall-Héroult process as the most important industrial application, is currently a major part of modern electrochemistry. In 1995 for example, the total world production was about 6.3 thousand metric tons of lithium, 339 thousand metric tons of magnesium, and 19.4 million metric tons of aluminium. It is clear that in order to use and to develop the high-temperature electrochemical technologies the knowledge in modern electrochemistry of molten salts is important. It was shown in the BRITE/Euram II Project (Contract no. BRE2.CT93.0447) that electrochemical investigation of the molten salt catalytic media can help to understand the mechanism of catalytic reaction.

**Molten Salt Catalysis**

First publications on molten salt catalysis appeared more than 100 years ago and now processes with molten salt catalysts (molten metal halides and oxides and their mixtures: ZnCl₂, AlCl₃, CuCl₂, V₂O₅, MoO₃ etc.) are widely used in the industrial production of isoparaffins, chlorination of hydrocarbons, gasification of coal etc. It was also proved that the catalytic SO₂ oxidation during the sulfuric acid production takes place in a film consisting of V₂O₅ in molten alkali pyrosulfates. Molten salt catalysis is the usual type of homogeneous catalytic reaction. However molten salt catalysts have the peculiar properties which make them sometimes the only possibility to synthesize definite organic or inorganic compounds due to: 1. High working temperatures. 2. Absence of water. 3. High concentration of catalyst. 4. Wide acid-base range. 5. High thermal and electric conductivity. Study on the mechanism of the catalytic SO₂ oxidation was the main aim of BRITE/Euram II Project Contract no. BRE2.CT93.0447. In this investigation the V₂O₅ - M₂S₂O₃ (M is alkali metal) melt was used as a model of the catalyst for the sulphuric acid production. It was shown that electrochemical techniques can be a powerful tool in the study of the mechanism of a catalytic reaction.
Supervisor:
Ridder, Carsten (Ekstern)
Main Supervisor:
Hansen, Elo Harald (Intern)
Examiner:
Frisvad, Jens Christian (Intern)
Gundersen, Vagn (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Sektorministerium, Stip-SU
Project: PhD

Faseligevægte, mikrostruktur og domæner i lipidmembraner.

Department of Chemistry
Period: 01/08/1993 → 02/10/1996
Number of participants: 4
Phd Student:
Lemmich, Jesper (Intern)
Supervisor:
Ipsen, John Hjorth (Intern)
Main Supervisor:
Mouritsen, Ole G. (Intern)
Examiner:
Dahl, Jens Peder (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-Su Stipendium, Eksperiment
Project: PhD

Glykosidsyntese antistoffer

Department of Chemistry
Period: 01/08/1993 → 14/01/1996
Number of participants: 5
Phd Student:
Tagmose, Tina Møller (Intern)
Supervisor:
Bols, Mikael (Ekstern)
Main Supervisor:
Lundt, Inge (Intern)
Examiner:
Jensen, Søren Rosendal (Intern)
Pedersen, Erik Bjerregaard (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: DTU-Su Stipendium, Eksperiment
Project: PhD

Metalloproteineres totalsyntese, spektralegenskaber og elektrontransport.

Department of Chemistry
Period: 01/08/1993 → 01/01/2007
Number of participants: 2
Phd Student:
Iversen, Gitte (Intern)
Main Supervisor:
Ulstrup, Jens (Intern)
Financing sources
Source: Internal funding (public)
Name of research programme: DTU-Su Stipendium, Eksperiment
Project: PhD

Statistisk mekanik af grænseflader i bløde stoffer

Department of Chemistry
Period: 01/07/1993 → 23/05/1997
Number of participants: 5
Phd Student:
Hansen, Per Lyngs (Intern)
Supervisor:
Ipksen, John Hjorth (Intern)
Main Supervisor:
Mouritsen, Ole G. (Intern)
Examiner:
Fogedby, Hans C. (Ekstern)
Hansen, Flemming Yssing (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsstip.-SU, Eksp
Project: PhD

Clay Minerals
The far-sighted purpose of the project is to develop a model to describe interaction between surfaces of minerals and molecules of any kind in the aqueous phase surrounding the mineral. The present ongoing research aims at modelling known crystal structures of montmorillonites and related minerals by optimising parameters of potential energy functions derived from ab initio studies. Modelling studies include sorption of water, ions and organic compounds.

Department of Chemistry
Period: 01/04/1993 → 31/12/2003
Number of participants: 2
Project participant:
Teppen, Brian (Ekstern)
Project Manager, organisational:
Rasmussen, Kjeld (Intern)

Financing sources
Source: Unknown
Name of research programme: Uendt
Amount: 112,000.00 Danish Kroner
Project

Undersøgelse af forekomst af detergenter og andre overfladeaktive stoffer i indemiljøet og sådanne stoffers indvirkning på indeklimaet

Department of Chemistry
Period: 01/04/1993 → 03/02/1997
Number of participants: 4
Phd Student:
Vejrup, Karl Ventzel (Intern)
Main Supervisor:
Madsen, Jørgen Øgaard (Intern)
Examiner:
Nielsen, Peter A. (Ekstern)
Svensmark, Bo (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskerakademiets Samfinansier
**Uorganisk sporeelementanalyse med ICP/MS.**

Department of Chemistry  
Period: 01/04/1993 → 27/02/1997  
Number of participants: 4  
Phd Student:  
Behrens, Annette (Intern)  
Main Supervisor:  
Hansen, Elo Harald (Intern)  
Examiner:  
Haraldsson, Conny (Ekstern)  
Mosbæk, Hans (Intern)

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: Forskerakademiets Samfinansier  
Project: PhD

**Anode Materials for Metal Hydride Batteries**

The aim is to develop new hydrogen storage alloys. The alloys are to be used as active material in the negative electrode of nickel metal hydride batteries (NiMH). State-of-the-art for NiMH is intermetallic compounds based on rare earth elements. These are developed from LaNi5. CaNi5 has the same structure and comparable hydrogen storage properties. If suitable electrode materials can be developed based on CaNi5, there is a potential for cheaper materials with a higher capacity. Intermetallics based on CaNi5 with partial substitutions are prepared and tested during the project. The hydrogen storage alloys are prepared from the elements by mechanical alloying in a planetary ball mill. After milling for several hours nanocrystalline intermetallics or amorphous alloys are formed. The alloys are characterized by X-ray powder diffraction before and after annealing in inert atmosphere. The hydrogen storage capacity is measured by gas absorption and the electrochemical properties are tested in half cells.

Department of Chemistry  
Period: 08/02/1993 → 30/04/1997  
Number of participants: 5  
Project participant:  
Berg, Rolf W. (Intern)  
Jensen, Jens Oluf (Intern)  
Hjuler, Hans Aage (Ekstern)  
Hennesø, Erik (Ekstern)  
Bjerrum, Niels J. (Intern)  
Project: PhD

**Flercentrede bakterielle hæmoproteiners elektrotransport**

Department of Chemistry  
Period: 01/02/1993 → 23/04/1996  
Number of participants: 3  
Phd Student:  
Karlsson, Jens-Jakob (Intern)  
Main Supervisor:  
Ulstrup, Jens (Intern)  
Examiner:  
Nielsen, Hans Toftlund (Ekstern)

**Financing sources**  
Source: Internal funding (public)  
Name of research programme: DTU-Su Stipendium, Eksperiment  
Project: PhD
Kohærente og “Squeezede” for det elektromagnetiske felt, atomer og små molekyler

Department of Chemistry  
Period: 01/02/1993 → 12/11/1996  
Number of participants: 4  
Phd Student:  
Jørgensen, Thomas Godsk (Intern)  
Main Supervisor:  
Dahl, Jens Peder (Intern)  
Examiner:  
Avery, John (Ekstern)  
Henriksen, Niels Engholm (Intern)  

Finance sources  
Source: Internal funding (public)  
Name of research programme: DTU-Su Stipendium, Eksperiment  
Project: PhD

Metoder til generering af kulstof-kulstof bindinger i derivatiserede aldonolactoner

Department of Chemistry  
Period: 01/02/1993 → 09/07/1996  
Number of participants: 3  
Phd Student:  
Horneman, Anne Marie (Intern)  
Main Supervisor:  
Lundt, Inge (Intern)  
Examiner:  
Pedersen, Christian (Ekstern)  

Finance sources  
Source: Internal funding (public)  
Name of research programme: DTU-Su Stipendium, Eksperiment  
Project: PhD

Selvorganisering i diffusivt drevne systemer med intrinisk ikke-linearitet.

Department of Chemistry  
Period: 01/02/1993 → 08/01/1996  
Number of participants: 5  
Phd Student:  
Gilhøj, Henriette (Intern)  
Supervisor:  
Scott, Alwyn C. (Intern)  
Main Supervisor:  
Mouritsen, Ole G. (Intern)  
Examiner:  
Fogedby, Hans C. (Ekstern)  
Hansen, Flemming Yssing (Intern)  

Finance sources  
Source: Internal funding (public)  
Name of research programme: DTU-Su Stipendium, Eksperiment  
Project: PhD

Bioinorganic Chemistry  
Multifarious and sophisticated functions in the biological nature are associated with metal atoms. Striking examples are dioxygen transport and storage by hemoglobin and myoglobin, the biological nitrogen and sulphur cycles, biomineralization, or photosynthesis and respiration. The function of more than a third of all proteins is thus crucially determined by metals such as calcium, magnesium, iron, copper, zinc and molybdenum, but many other biological functions including all phases of DNA/RNA replication and transcription, macromolecular folding etc. are also associated with metals. The chemistry of metals in biological systems constitutes the new interdisciplinary science bioinorganic chemistry, which is rooted in inorganic chemistry but with broad interfaces to biochemistry, biophysics, and other sciences.
Fundamental research is directed towards biological structure and function with technological and biotechnological perspectives for example in environmental science, metals in medicine, industrial catalysts, microbiological metal extraction, sensors, and molecular nanoscale science. Bioinorganic chemistry at Technical University of Denmark is centred at Department of Chemistry, with broad national and European networks. The research is supported by the Danish Technical Science Research Council, and by the European Union. Research organization, and recent results are detailed below.

Department of Chemistry
University of Copenhagen
A. N. Frumkin Institute of Electrochemistry

Period: 01/01/1993 → …
Number of participants: 14
Project participant: Iversen, Gitte (Intern)
Jespersen, Lise-Lotte (Intern)
Andersen, Niels Højmark (Intern)
Jensen, Thomas Jon (Intern)
Friis, Esben P. (Intern)
Nielsen, Jens Ulrik (Intern)
Hansen, Allan Glargaard (Intern)
Zhang, Jingdong (Intern)
Chi, Qijin (Intern)
Christensen, Hans Erik Mølager (Intern)
Led, Dr. J.J. (Ekstern)
Kharkats, Prof. Yu.I. (Ekstern)
Kuznetsov, Prof. A.M. (Ekstern)

Project Manager, organisational: Ulstrup, Jens (Intern)

Financing sources
Source: Udenfor rammen
Name of research programme: Ukendt
Amount: 250,000.00 Danish Kroner
Source: Udenfor rammen
Name of research programme: Ukendt
Amount: 50,000.00 Danish Kroner
Source: Udenfor rammen
Name of research programme: Ukendt
Amount: 50,000.00 Danish Kroner

Project

Complex and Redox Chemistry in Molten Halides
Chloride, fluoride and mixed chloride-fluoride melts are currently investigated by Raman and IR spectroscopy and by electrochemical methods like cyclic voltammetry and square wave voltammetry. The scope of the project is to clarify the complex and oxidation reactions taking place in melts, that can be applied as molten salt baths for plating with corrosion and abrasion resistant layers.

Department of Chemistry

Period: 01/01/1993 → …
Number of participants: 8
Project participant: Berg, Rolf W. (Intern)
Bjerrum, Niels J. (Intern)
Gillesberg, Bo (Intern)
Polyakov, E. (Ekstern)
Polyakova, L. (Ekstern)
Lantelme, F. (Ekstern)
Picard, G. (Ekstern)

Project Manager, organisational:
Macrocyclic ligands and their coordination compounds
Bio-inorganic chemistry (or bio-coordination chemistry) is a rapidly growing field, which can be divided into studies of the native systems and the study of model systems. The project includes solely model systems, and the purpose is to synthesize macrocyclic coordination compounds followed up by investigations of the reactivity of these compounds with a special reference to reactions, which can elucidate the relationships within the analogous native existing compounds (enzymes). A detailed knowledge of the structure of the compounds is necessary for this purpose. The project consists of two parts: a. Tetrahedral coordinated bi- and tricyclic ligands. b. Bis- and tris-macrocyclic ligands. Special designed macrocyclic ligands have been synthesized and their structures have been examined. The research is carried out in cooperation with chemists at the Royal Veterinary and Agricultural University, Copenhagen.

Molten Carbonate Fuel Cells (MCFC)
One of the major problems for operating molten carbonate fuel cells is the corrosion of metal oxide electrodes. In this connection the dissolution of various oxides of transition metals in molten Li-K carbonates has been studied. Electrochemical behavior of several metal electrodes (Au, Ag, Cu, Fe, Al, Ti, Cr etc.) has been studied. A novel method for corrosion protection of metals in molten alkali carbonates is also developed by deposition of an AlN-TiN layer.

Barner, Jens H. Von (Intern)
Project

Kompleks og redoxkemi i saltsmeltebade til ovrfladebehandlingsprocesser
Department of Chemistry
Period: 01/01/1993 → 27/02/1997
Number of participants: 4
Phd Student:
Andersen, Kjeld Bøhm (Intern)
Main Supervisor:
Bjerrum, Niels J. (Intern)
Examiner:
Hjuler, Hans Aage (Intern)
Skou, Eivind Morten (Ekstern)

Financing sources
Source: Internal funding (public)
Name of research programme: Forskningsrådsstip.-SU, Eksp
Project: PhID

Royal Veterinary and Agricultural University
Period: 01/01/1993 → ...
Number of participants: 2
Project participant:
Springborg, Reader Johan (Ekstern)
Project Manager, organisational:
Søtofte, Inger (Intern)

Ansaldo CLC
Foundation for Research and Technology-Hellas
Period: 01/01/1993 → 31/12/1998
Number of participants: 2
Project participant:
Li, Qingfeng (Intern)
Project Manager, organisational:
Bjerrum, Niels J. (Intern)
Trace metal analysis in soil, waste water and drinking water by potentiometric stripping analysis (PSA) methods
The aim of this project is to obtain methods for differentiation between poisonous and non-poisonous metallic species in the environment. In contrast to conventional PSA, where the reoxidation of the prereduced/preconcentrated analytes in the mercury film of the working electrode is based on the use of mercury ions, this project is concerned on finding alternative means of oxidation thereby obviating the use of mercury ions and hence make the method more environmentally acceptable. This is much in demand, because the method as such is a simple, inexpensive and expedient approach for trace level determinations as compared to the more costly optical procedures commonly applied.

Department of Chemistry

Adsorption of hydrocarbons in chalk reservoirs
With the aim of understanding the governing principles for wettability of hydrocarbon reservoirs, we study the adsorption of polar hydrocarbons on chalk and on selected minerals from a hydrocarbon as well as an aqueous phase. The adsorption is studied on powders using a batch method, and the obtained adsorption isotherms form the basis for interpretation.

Department of Geology and Geotechnical Engineering
Department of Chemistry
Department of Environmental Engineering

RISØ
Period: 01/12/1992 → 27/06/1996
Number of participants: 4
Project participant:
Madsen, Lene (Intern)
Engell, John Emil (Intern)
Grøn, Christian (Ekstern)
Project Manager, organisational:
Fabricius, Ida Lykke (Intern)

Model studies of random surfaces, interfaces, and microemulsions
Department of Chemistry
Period: 01/12/1992 → 14/01/1997
Number of participants: 3
Phd Student:
Dammann, Bernd (Intern)
Main Supervisor:
Keramiske membranfiltere

Department of Chemistry
Period: 01/11/1992 → 30/04/1997
Number of participants: 2
Phd Student:
Tranto, Janne (Intern)
Main Supervisor:
Høj, Jakob Weiland (Intern)

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

Inelastic Neutron Scattering in Saccharides and Model Compounds

Work was continued on the interpretation of the first neutron spectra obtained on a series of monosaccharides, disaccharides and compounds acting as saccharide models. The work is carried out during visits to the ISIS facility at Rutherford Appleton Laboratory. Progress is made in interpretation of the very complicated spectrum of trioxan, and on the adaptation of the normal coordinate program to handle lower symmetry and larger substances. It is the intention to couple INS spectra to the optimisation of potential energy function parameters done with CFF, the Consistent Force Field.

Department of Chemistry
Period: 01/10/1992 → 31/12/2003
Number of participants: 2
Project participant:
Tomkinson, John (Ekstern)
Project Manager, organisational:
Rasmussen, Kjeld (Intern)

Mekanismer for metalloproteiners intermolekylære og elektrokemiske elektrontransport

Department of Chemistry
Period: 01/09/1992 → 27/02/1996
Number of participants: 3
Phd Student:
Thuesen, Marianne Hallberg (Intern)
Main Supervisor:
Ulstrup, Jens (Intern)
Examiner:
Hammershøj, Anders (Ekstern)

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

Biosyntese af iridoid glucosider, hvor C-10 mangler

Department of Chemistry
Period: 01/08/1992 → 29/06/1995
Number of participants: 3
Phd Student:
Frederiksen, Lotte Boe (Intern)
Supervisor:
Damtoft, Søren (Ekstern)
Main Supervisor:
Jensen, Søren Rosendal (Intern)

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

Nye elektroder- og elektrolytmateriale til højtemperatur faststofoxidbrændselsceller
Department of Chemistry
Period: 01/04/1992 → 23/02/1995
Number of participants: 2
Phd Student:
Ranløv, Jens (Intern)
Main Supervisor:
Nielsen, Kurt (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Gammel Ordning - Blandet Finan
Project: PhD

Teoretisk bestemmelse af UNIFAC-parametre
Department of Chemistry
Period: 01/04/1992 → 18/04/1995
Number of participants: 2
Phd Student:
Jonsdottir, Svava Osk (Intern)
Main Supervisor:
Rasmussen, Kjeld (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Gammel ordning u/skema-SU
Project: PhD

Integreret studium af molekylære vekselvirkninger i lipidmembraner
Department of Chemistry
Period: 01/02/1992 → 03/11/1994
Number of participants: 3
Phd Student:
Callisen, Thomas Hønger (Intern)
Supervisor:
Laursen, Ib (Intern)
Main Supervisor:
Mouritsen, Ole G. (Intern)

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

Termoelektroska effekter i fastoxid brancleceller
Department of Chemistry
High Performance Coating Materials for Application in Corrosive and Abrasive Environments

The main object of this project is to develop processes for electrolytical deposition of corrosion resistant coatings of niobium and tantalum from alkali fluoride melts (FLINAK). The aim is to protect components used in chemical industry against corrosion. The work is concentrated partly towards coating of objects of steel with a high complexity of geometry, as well as basic scientific studies of the electrochemistry and complex formation in the molten electrolytes. A number of tantalum coated steel objects have been produced for field tests in Danish industry. The project is carried out in close cooperation with Danfoss A/S.

Department of Chemistry

Minor organic compounds

In connection with selective synthesis it is important to know the conformation of the molecules. The crystal structure of a number of compounds has been determined.

Department of Chemistry

Teknisk Keramik’s egenskaber som funktion af tilsætning af SiO2, MgO, FeO og MnO etc.

Department of Chemistry

Financing sources

Source: Internal funding (public)
Name of research programme: Nordisk finansiering
Project: PhD
Electron and proton transfer dynamics of metalloproteins

Department of Chemistry
Period: 01/09/1990 → 04/01/1994
Number of participants: 2
PhD Student:
Hammerstad, Jan Meldtoft (Intern)
Main Supervisor:
Ulstrup, Jens (Intern)

Financing sources
Source: Internal funding (public)
Name of research programme: Gammel ordning u/skema-SU
Project: PhD

Conducting Polymers
Polymers with alternating (conjugated) single and double bonds have unusual electronic properties that are normally not associated with polymer materials. By oxidation or reduction, mobile electronic defects may be introduced on the conjugated backbone, rendering these polymers electronic conductors. In extreme cases, electronic conductivity better than copper (by weight) have been reported. The introduction of charges on the polymer backbone requires that compensating counter charges are introduced into the polymer matrix. This process is often referred to as "doping", but is conceptually identical to an intercalation reaction. Conducting polymers may therefore be useful in the same kinds of applications as described for intercalation materials: Rechargeable batteries, electrochromic displays showing controllable color change, as well as in sensors. We have characterised a number of conducting polymers and demonstrated how the analogy to intercalation may help in the understanding of the complex behaviour of these systems. One important difference between inorganic intercalation materials and conducting polymers is the lack of perfection of the polymer structure. High concentrations of defects may be present in the chemical bonds making up individual polymer chains, and the stacking of these chains into a "crystal lattice" is far from uniform. By careful control of the synthesis of poly-pyrrrole, we have demonstrated how the degree of perfection of the polymer backbone greatly influences the physical and electrochemical properties of the polymer. Polymers are relative soft materials, and the doping process may lead to significant changes in the dimensions of conducting polymers. We are presently investigating the exploitation of this electro-chemo-mechanical effect in mechanical actuators - "artificial muscles". The aim is to be able to precisely control position and force by the application of a small (
may help in the understanding of the complex behaviour of these systems. One important difference between inorganic intercalation materials and conducting polymers is the lack of perfection of the polymer structure. High concentrations of defects may be present in the chemical bonds making up individual polymer chains, and the stacking of these chains into a “crystal lattice” is far from uniform. By careful control of the synthesis of poly-pyrrole, we have demonstrated how the degree of perfection of the polymer backbone greatly influences the physical and electrochemical properties of the polymer. Polymers are relative soft materials, and the doping process may lead to significant changes in the dimensions of conducting polymers. We are presently investigation the exploitation of this property in mechanical actuators - "artificial muscles".

Department of Physics
Department of Chemistry
Risø National Laboratory for Sustainable Energy
Danfoss A/S
Period: 01/01/1990 → 31/12/1996
Number of participants: 3
Project participant:
West, Keld (Intern)
Zachau-Christiansen, Birgit (Intern)

Project Manager, organisational:
Skaarup, Steen (Intern)

Corrosion Measurement by Titration, Applications and Development
Corrosion Measurement by Titration has been developed as a faster, more reliable and quantitative alternative to current technical test methods. Frequently this method gives results differing from the results of electrochemical measurements. Analysis of these differences and the conditions leading to different results has revealed important details in the basic reaction mechanisms of metal dissolution.

Department of Chemistry
Period: 01/01/1990 → 30/06/2002
Number of participants: 1
Project Manager, organisational:
Bech-Nielsen, Gregers (Intern)

Dynamical Symmetry
A symmetry that couples the kinetic and potential energy parts of the Hamiltonian is known as a dynamical symmetry. The most studied dynamical symmetry is probably that associated with the Kepler problem. In the non-relativistic Kepler problem, the symmetry manifests itself through the so-called Runge-Lenz vector which is a constant of the motion - both in classical mechanics and in quantum mechanics. In the relativistic Kepler problem, the Runge-Lenz vector ceases to be a constant of the motion. The removal of the dynamical symmetry is, however, not complete. The relativistic symmetry is accounted for by means of a constant of the motion originally introduced by Johnson and Lippmann. The present project is concerned with salient aspects of both the non-relativistic and the relativistic Kepler problem. The project is partly financed by a grant from The Danish Natural Sciences Research Council (SNF).

Phase Space Formulation of Quantum Mechanics
Quantum-mechanical descriptions that operate in phase space have proved very useful, both for the description of particle motion and for the description of the quantized electromagnetic field. The project includes: 1. Foundation of phase-space representations; 2. Group-theoretical aspects; 3. The dual nature of phase-space representations; 4. Wavefunctions in phase space; 5. Dynamical equations for phase-space distributions; 6. Analytical and numerical generation of phase-space distributions for oscillators, atoms and molecules; 7. Applications in molecular dynamics; 8. Applications in spectroscopy; 9. Coherent and squeezed states of the electromagnetic field. The project is partly financed by a grant from
Solid Oxide Fuel Cell Materials and Kinetics
The project is a subproject in the danish DK-SOFC Programme. In Solid Oxide Fuel Cells (SOFC) operating at 1000 degrees C non-stoichiometric oxide are applied as electrode and interconnect materials. The electronic and ionic transport properties of these materials depend on the oxygen stoichiometry and will therefore change with the load in SOFC operation. In this project the oxygen stoichiometry of SOFC related materials is determined as function of oxygen partial pressure, or electrode potential. The measurements are performed by Slow Potential Scan technique on oxygen pumping cells in the temperature range 800-1000 degrees C. The SOFC electrode reactions proceed along the three phase boundary where the gas phase is in contact with the electrode and the electrolyte. The reaction mechanisms, including problems like the width of the reaction zone, is studied by electrochemical techniques as linear sweep voltammetry and impedance spectroscopy on electrodes of simple geometry, point electrodes combined with model calculations.
Lipases in Organic Synthesis

Running tests of the usefulness of industrial lipases in organic synthesis. Dicarboxylic Acid Monoesters using Candida antarctica Lipase B (Novo Nordisk). Resolution of Aliphatic Hydroxysubstituted Esters using Candida antarctica Lipase B (Novo Nordisk). The Resolution implicate Lipase catalyzed Esterification of the Hydroxy Group or Hydrolysis of the Ester Function. Chiral and Achiral Cyclic Carboxylic Esters as Substrates for Candida antarctica Lipase B. Cyclohexane and Cyclopentane Carboxylic Acid Systems proved good Substrates, Cyclobutane and Cyclopropane Systems much less so. Some cyclic Chiral Acids were Resolved very satisfactorily using this Technique. Substrate Specificity of Candida antarctica Lipase A. In collaboration with Morten W. Christensen and Ole Kirk, Novo Nordisk (project coordinators). Esterification of a number of Primary and Secondary Alcohols with Fatty Acids was investigated, mainly by Competition Experiments. Investigation of Substrate Specificity of Candida antarctica Lipase B modified by Protein Engineering; three different Substitutions of Amino Acids in the Lipase was tried (Project coordinator: Ole Kirk, Novo Nordisk). Two of the Modified Lipases were tested in this Dept. for Enantioselectivity in the Esterification of certain Racemic Secondary Alcohols. Preparative Resolution of Chiral Alcohols catalyzed by Candida antarctica Lipase B using Hydrolysis of a corresponding Ester or Esterification of the Alcohol. A number of highly successful Resolutions of secondary Alcohols of Diverse Structures have been carried out. Regioselective Acylations of selected carbohydrate derivatives catalyzed by Candida antarctica Lipase B. Regioselective Acylations of Glycerol catalyzed by Candida antarctica Lipase B and other Novo Nordisk Lipases.

Department of Organic Chemistry

Crystallography

Crystallographic studies is a major research field of the Structural Chemistry Group at the Department of Chemistry. A large number of crystal structure determinations by X-ray crystallographic methods have been carried out. Two single-crystal diffractometers as well as one powder diffractometer are in use. The newest instrument is a Siemens/Bruker SMART diffractometer with a fast CCD area detector which makes it possible to measure many diffraction intensities within a short time. Data interpretation and representation of structural results involves extensive use of crystallographic computer software. Several crystallographic databases are at disposal. The crystallographic studies are integral parts of several specific projects listed separately. Acquisition of instruments as well as running expenses are supported by grants from the Danish Natural Science Research Council.

Department of Chemistry

Fungal metabolites


Department of Organic Chemistry
Department of Chemistry
Novo Nordisk A/S
Period: 01/01/1988 → 31/12/2000
Number of participants: 3
Project participant:
Kjær, Dana (Intern)
Breinholt, Jens (Ekstern)
Project Manager, organisational:
Kjær, Anders (Intern)

MEMPHYS -- Membrane and Statistical Physics Group
Principal Areas of Research: Statistical mechanics and thermodynamics, computer simulation techniques, phase transitions and critical phenomena, calorimetry, fluorescence spectroscopy, electron-spin resonance spectroscopy, biomembrane physics and chemistry, physical chemistry of surfaces and interfaces, soft matter, materials science. Phase transitions in solids and fluids, Monte Carlo methods, liquid crystals, overlayers on solid surfaces, domain–growth kinetics, grain growth and grain boundaries, interfaces and melting, solidification, fractals and pattern formation, transport phenomena, ceramic high–temperature superconductors, polymers, random surfaces, lipid monolayers and bilayers, biological membranes, lipid membranes and liposomes incorporated with cholesterol, proteins, polypeptides, drugs and insecticides, phospholipase action. Visiting scientists in 1999: Prof. Martin J. Zuckermann (McGill) Prof. Robert Cantor Dr. James Polson (McGill) Dr. Thomas Heimburg (MPI, Goettingen) During the period the project has received financial support from the following sources: The Danish Natural Science Research Council The Danish Technical Science Research Council The Danish Medical Research Council Canadian Institute for Advanced Research Carlsberg Foundation The Danish Research Academy The Hasselblad Foundation

Department of Chemistry
Period: 01/07/1985 → 31/12/2000
Number of participants: 18
Project participant:
Ipsen, John Hjorth (Intern)
Besold, Gerhard (Intern)
Miao, Ling (Intern)
Dammann, Bernd (Intern)
Sabra, Mads Christian (Intern)
Trandum, Christa (Intern)
Jacobsgaard, Helle E. Hjorting (Intern)
Klausen, Jette (Intern)
Nielsen, Lars Kildemark (Intern)
Høyrup, Lise Pernille Kristine (Intern)
Vissing, Thomas (Intern)
Callisen, Thomas Hønger (Intern)
Vattulainen, Ilpo Tapio (Intern)
Jørgensen, Kent (Intern)
Westh, Peter (Intern)
Jensen, Morten Østergaard (Intern)
Kaasgaard, Thomas (Intern)
Project Manager, organisational:
Mouritsen, Ole G. (Intern)

Financing sources
Source: Unknown
Name of research programme: Ukendt
Amount: 600,000.00 Danish Kroner
Source: Unknown
Name of research programme: Ukendt
Amount: 1,360,000.00 Danish Kroner
Source: Unknown
Name of research programme: Ukendt
Fast Reactions in Solution

For many decades (1850-1920) the progress of chemical reactions as a function of time was only observable for relatively slow reactions (half-lives > seconds), where samples were taken from time to time and analysed by classical analytical methods. However, this group of (classical) reactions represents only a fraction of all reactions, and today we are able to study experimentally also the remaining group - the fast reactions - where systems with half-lives of the order of magnitude from milli- to pico- and even femto-seconds can be reached. In our research group we are primarily interested in measuring chemical reaction rates in the range of seconds to microseconds. We have access to experimental equipment such as stopped-flow and a relaxation spectrometer, the latter based on the temperature- and pressure-jump principle. Since proton transfer reactions - relating to acid-base catalysis - are often fast processes, our instruments are essential for the study of such systems and have for a long time formed the experimental basis for our research in this field. In focus at the moment are studies of: 1. Equilibria and kinetics of the hydration of simple dialdehydes, such as glyoxal and its derivatives. These compounds appear in all living cells (cell growth regulators), and a study of their fundamental physico-chemical reactions is important to a more complete understanding of their biological function. 2. The bema hapothle in acid base catalysis. A study of the interaction between free energy correlations parameters at different reaction sites, following formulations by W. P. Jencks. 3. Protonation of simple cryptands. The two nitogens are protonated at different rates and the molecules undergo drastic conformational changes, coupled to this protonation in a rather complicated way.

Department of Chemistry
University of Toronto
Period: 01/01/1985 → 31/12/1999
Number of participants: 2
Project participant:
McClelland, Robert A. (Ekstern)
Project Manager, organisational:
Sørensen, Poul Erik (Intern)

FIA and Chemometrics

This project focuses on the use of scanning detectors (primarily optical) for exploiting the (theoretical) infinite time-dependant data in the matrix, which any FIA-concentration gradient inherently represents, supplemented by application of advanced mathematical and statistical methods to resolve the spectral information, e.g., for simultaneous determination of several components. Previous Ph.D-projects include selective determination of rare earth elements by means of ICP-MS (in cooperation with Research Center Risø), and multivariate methods for the assessment of fundamental quality parameters for frozen fish. Additionally, published results comprize applications to potentiometric stripping analysis (PSA) and FIA-speciation procedures.

Department of Chemistry

Flow Injection Trace Metal Determinations and Speciation Procedures

These procedures are based on detection via atomic absorption spectrometry (AAS), that is, either flame-AAS, electrothermally heated AAS (ET-AAS), or hydride generation-AAS. Special emphasis is placed on designing on-line preconcentration techniques in order to reach the very low limits of detection required in modern environmental analyses and to obtain sufficient selectivity via separation of the measurand from interfering matrix constituents. The preconcentration techniques comprize the use of incorporated column reactors containing ion-exchangers, exploitation of on-line generation of non-polar complexes which subsequently are selectively extracted, or the use of filterless precipitation/coprecipitation, where the preconcentration in the latter instance is effected by adsorption on the inner wall of a knotted reactor and where the precipitate ensuingly is eluted by a discrete zone of eluent. The research activities in this field is currently (1999/2000) being supplemented with the acquisition of an Inductively Coupled Plasma Mass Spectrometry (ICP-MS) instrument, which promises to entail even lower limits of detection and enhanced selectivity of measurement.
Kinetic FIA-discrimination procedures with the aim of determining transient/metastable species of specific analytically interesting characteristics

Several chemical reactions proceed through intermediary steps, some of which might entail the formation of species of analytically interesting characteristics (such as species of particularly high molar absorptivities as compared to the ultimately generated end-products). Due to its inherent exact and reproducible timing, FIA is a very attractive vehicle to use to detect such species - especially if side reactions entail the formation of coproducts that can give rise to signals at the measurements conditions used.

Consistent Force Field

The Consistent Force Field, CFF, was developed here, based on the original work of Lifson and Warshel at the Weizmann Institute of Science in the late 1960es. The CFF is a tool with which you can develop force fields, in the sense that you can optimize the parameters of potential energy functions on several categories of data for molecules in gaseous and crystalline states. The imbedded methods allow for calculation of molecular properties such as conformations, vibrational
frequencies and thermodynamic functions. The integrated optimization facility is unique and fundamental to the CFF concept. The most important technical contributions from this group are: weighted Levenberg-Marquardt optimization, a crystal simulator using Ewald sums, and an interactive graphical interface to the optimization algorithm GOPT (Graphics Optimization Tool). The uniqueness of CFF is found in its optimization capabilities. At present CFF can optimize on bond lengths, valence angles, torsional angles, out-of-plane angles, non-bonded distances, unit cell dimensions, lattice energies, dipole moments, and vibrational frequencies. Applications of CFF are numerous: coordination compounds; saccharides; aluminosilicates; intermolecular interactions and phase equilibria.

Department of Chemistry

Period: 01/09/1979 → 31/12/2003

Number of participants: 1

Project Manager, organisational: Rasmussen, Kjeld (Intern)

Project

Intercalation - Reactions and Materials

Intercalation is the reversible insertion of mobile guests - ions or molecules - into an open host structure. These reactions are conducted under mild thermal conditions where rearrangements of the bonds in the host structure is prevented from kinetic reasons. Intercalation reactions may thus lead to labile products that could not be prepared by conventional equilibrium reactions. Intercalation of ions can be driven as an electrochemical process. As the density of guest ions can be very high, such reactions are the ideal basis for charge storage in secondary (rechargeable) batteries. For this purpose, we have studied and characterized lithium and sodium intercalation in large number of transition metal oxides and sulphides. The main emphasis is on the determination of variations of the voltage of intercalation electrodes with composition - and on understanding how this property depends on both structure and chemical composition of the host materials. The voltage-composition relationship is the property that determines the energy density of batteries based on intercalation materials. We have also investigated the kinetics of intercalation reactions, as well as the ability to withstand a large number of insertion-extraction (charge-discharge) cycles. Intercalation electrodes may be useful in other applications as well. We have studied colour changes in intercalation materials following lithium or hydrogen ion intercalation. Such materials may find use in electrochromic devices (displays). Likewise, we have studied the application of intercalation materials in sensors. Intercalation reactions are non-equilibrium reactions offering a high degree of simultaneous control of both structure and composition which will normally not be available through conventional equilibrium synthesis. We are presently trying to exploit this possibility in the synthesis of nano-composites made up by interpenetrating inorganic (ceramic) and organic (polymer) networks.

Department of Chemistry

Period: 01/10/1978 → …

Number of participants: 4

Project participant: Zachau-Christiansen, Birgit (Intern)

Skaarup, Steen (Intern)

Jacobsen, Torben (Intern)

Project Manager, organisational: West, Keld (Intern)

Project

Flow Injection Enzymatic Assays

This project is concerned at quantifying both substrates and enzyme activities, particularly with detection by optical means (UV/Vis, fluorometry, bio- and chemiluminescence), and including assays based on enzyme amplification schemes. Special emphasis is placed on devising generic systems, that is, FIA-systems which can be designed to serve as templates for a multitude of individual species.

Department of Chemistry

Period: 01/01/1978 → …

Number of participants: 1

Project Manager, organisational: Hansen, Elo Harald (Intern)

Project
Analytical Chemistry with special emphasis on the use of Flow Injection Analysis

Development and application of methods and procedures based on Flow Injection Analysis (FIA) - with analytical concept originally was developed by this group in the mid-70’es and about which over 10,000 papers since have been published world-wide in international scientific periodicals. This feat is not the least due to the adapability of FIA to virtually any type of detection device. Current projects comprize: Enzymatic assays; Trace metal determinations and speciation procedures with detection by atomic absorption spectrometry (AAS) and inductively coupled plasma mass spectrometry (ICP-MS); Kinetic FIA-descrimination procedures with the aim of determining transient/metastable species of specific analytically interesting characteristics; Trace metal analysis in soil, waste water and drinking water by potentiometric stripping methods; and determinations based upon the combination of FIA and chemometrics. The individual projects are briefly described separately in the attached subprojects.

Department of Chemistry

Period: 01/01/1975 → …
Number of participants: 6
Project participant:
Andersen, Jens (Intern)
Behrens, Annette (Intern)
Bechmann, Iben Ellegaard (Intern)
Thale, Eva Illum (Intern)
Johansen, Inge Marie (Intern)

Project Manager, organisational:
Hansen, Elo Harald (Intern)

Financing sources
Source: Unknown
Name of research programme: Ukendt
Amount: 47,392.00 Danish Kroner
Source: Unknown
Name of research programme: Ukendt
Amount: 30,000.00 Danish Kroner
Source: Unknown
Name of research programme: Ukendt
Amount: 76,239.00 Danish Kroner

Project

Saccharide Modelling

In 1996 a new potential energy function for saccharides, PEF95SAC, was finished. Its parameters are optimised on experimental data for alcohols, ethers and saccharides: gas phase stucture from electron diffraction corrected to r(z), crystal stucture from neutron diffraction, and vibrational spectra in the gas phase. The validity of the new function was checked on structural, spectral and thermodynamic data not included in the optimisation. In 1997 it was tested together with 19 other functions in an international collaborative effort published in 1999. A study of the history of development of force fields for saccharides, including a new mapping of the conformational space of sucrose, and concluding with questions for the future, was published in 1999. Collaboration on development of saccharide force fields based on quantum chemical studies has been initiated with colleagues in the USA.

Department of Chemistry

Period: 01/09/1973 → 31/12/2003
Number of participants: 2
Project participant:
Momany, Frank A. (Ekstern)

Project Manager, organisational:
Rasmussen, Kjeld (Intern)

Financing sources
Source: Unknown
Name of research programme: Ukendt
Amount: 112,000.00 Danish Kroner

Project

Activities:
2018 Pacific Conference on Spectroscopy and Dynamics
Period: 25 Jan 2018 → 28 Jan 2018
René Wugt Larsen (Participant)
Department of Chemistry
Degree of recognition: International

Related event
2018 Pacific Conference on Spectroscopy and Dynamics
25/01/2018 → 28/01/2018
San Diego, United States
Activity: Attending an event › Participating in or organising a conference

European inorganic chemistry conference
Period: 2017 → …
Susanne Mossin (Organizer)
Center for Hyperpolarization in Magnetic Resonance
Department of Chemistry
Centre for Catalysis and Sustainable Chemistry
Organic Chemistry

Description
Organizer of international conference
Degree of recognition: International

Related event
European inorganic chemistry conference
02/07/2017 → 05/07/2017
Copenhagen, Denmark
Activity: Attending an event › Participating in or organising a conference

Bioenergy conversion and storage systems: from conventional electrochemical cells to hybrid bioelectronic devices
Period: 6 Dec 2017
Dmitrii Pankratov (Invited speaker)
Department of Chemistry
NanoChemistry
Documents:
Abstract

Related event
DTU Sustain 2017
06/12/2017 → 06/12/2017
Kgs. Lyngby, Denmark
Activity: Talks and presentations › Conference presentations

DTU Sustain 2017
Period: 4 Dec 2017
Yingying Tang (Organizer)
Department of Chemistry
NanoChemistry
Degree of recognition: National
Documents:
Sustain DTU Abstract_Version 2_Yingying Tang
Related event

**DTU Sustain 2017**
06/12/2017 → 06/12/2017
Kgs. Lyngby, Denmark
Activity: Attending an event › Participating in or organising a conference

**3D Graphene-Glucose Oxidase Bioanodes for Enzymatic Biofuel Cells**
Period: 27 Nov 2017 → 28 Nov 2017
Jing Tang (Speaker)
Rebecka Maria Larsen Werchmeister (Other)
Jingdong Zhang (Other)
Department of Chemistry
NanoChemistry
Organic Chemistry
Documents:
Program Luckenwalde 2017-final

Related event

**PhD Workshop on Bioanalysis**
27/11/2017 → 28/11/2017
Postdam, Germany
Activity: Talks and presentations › Conference presentations

"Application of Scanning Probe Microscopy in Bioelectrochemistry"
Period: 27 Nov 2017 → 28 Nov 2017
Jingdong Zhang (Guest lecturer)
Department of Chemistry
NanoChemistry
Organic Chemistry

Description
PhD Workshop on Bioanalysis, University of Potsdam, Germany

Related external organisation

**University of Potsdam**
Germany
Activity: Talks and presentations › Conference presentations

**Go with the flow into spectroscopy: Selective reduction and oxidation of nitric oxide.**
Period: 9 Nov 2017
Susanne Mossin (Invited speaker)
Center for Hyperpolarization in Magnetic Resonance
Department of Chemistry
Centre for Catalysis and Sustainable Chemistry
Organic Chemistry

Description
Invited talk a the annual assembly

Related external organisation

**Danish Chemical Society, Inorganic Section**
Universitetsparken 5, 2100, KBH Ø, Denmark
Activity: Talks and presentations › Conference presentations

**Journal of Chemical Theory and Computation (Journal)**
Period: 8 Nov 2017
Sonia Coriani (Reviewer)
Department of Chemistry
Degree of recognition: International

**Related journal**
Journal of Chemical Theory and Computation
1549-9618
Central database

Activity: Research › Peer review of manuscripts

**Developing Theoretical Beamlines for Modern Experiments**
Period: 3 Nov 2017
Sonia Coriani (Invited speaker)
Department of Chemistry

**Related event**
Fall Meeting of the Division for Theoretical Chemistry 2017 of the Danish Chemical Society
03/11/2017 → 03/11/2017
Copenhagen, Denmark
Activity: Talks and presentations › Conference presentations

**Supercapacitive bioelectrochemical solar cells using thylakoid membranes and carbon nanotubes**
Period: 13 Oct 2017
Dmitrii Pankratov (Speaker)
Department of Chemistry
NanoChemistry
Degree of recognition: International
Documents:
Abstract GKS

**Related event**
2nd Gerischer-Kolb Symposium: Modern Aspects of Bioelectrochemistry International Bunsen Discussion Meeting
11/10/2017 → 13/10/2017
Günzburg/Donau, Germany
Activity: Talks and presentations › Conference presentations

**The Au-S bond in biomolecular adsorption and electrochemical electron transfer**
M.J. Ford (Other)
N.S. Hush (Other)
S. Marcuccio (Other)
J.R. Reimers (Other)
Jens Ulstrup (Invited speaker)
Jingdong Zhang (Other)
Department of Chemistry
NanoChemistry
Organic Chemistry

Description
2nd Gerischer-Kolb Symposium, Modern Aspects of Bioelectrochemistry, International Bunsen Discussion Meeting, Schloss Reisensburg, Germany, October 11 - 13, 2017
Degree of recognition: International
Documents:
AbstractGerischer_KolbOct2017

Related external organisation
University of Ulm
Ulm, Germany
Activity: Talks and presentations › Conference presentations

Local & ultrafast spectroscopies by coupled cluster methods
Period: 10 Oct 2017
Sonia Coriani (Invited speaker)
Department of Chemistry
Degree of recognition: International
Links:
http://www.anorg.chem.uu.nl/FXS2013/FXS2017participants.htm (Link to participant list and abstracts)

Related event
Workshop on Fundamental Aspects of X-ray Spectroscopies
09/10/2017 → 11/10/2017
Utrecht, Netherlands
Activity: Talks and presentations › Conference presentations

Workshop on Fundamental Aspects of X-ray Spectroscopies
Period: 9 Oct 2017 → 11 Oct 2017
Sonia Coriani (Participant)
Department of Chemistry
Degree of recognition: International
Links:
http://www.anorg.chem.uu.nl/FXS2013/FXS2017.htm (Conference website)

Related event
Workshop on Fundamental Aspects of X-ray Spectroscopies
09/10/2017 → 11/10/2017
Utrecht, Netherlands
Activity: Attending an event › Participating in or organising a conference

PhD opponent
Period: 29 Sep 2017
Sonia Coriani (External examiner)
Department of Chemistry
Degree of recognition: International
Activity: Examinations and supervision › External examination

Differentiating between exchange sites in small-pore zeolites by in-situ EPR
Period: Aug 2017 → …
Susanne Mossin (Other)
Center for Hyperpolarization in Magnetic Resonance
Department of Chemistry
"Developing Theoretical "Beamlines" for Modern Experiments"
Period: 31 Aug 2017
Sonia Coriani (Invited speaker)

Links:
http://www.watoc2017.com (Conference website)

The 11th Triennial Congress of the World Association of Theoretical and Computational Chemists
Period: 27 Aug 2017 → 1 Sep 2017
Sonia Coriani (Participant)

Links:
http://www.watoc2017.com/ (Conference websit)
"Exploring local and ultrafast spectroscopic effects by ab initio methods"
Period: 24 Aug 2017
Sonia Coriani (Invited speaker)
Department of Chemistry
Degree of recognition: International

Related event
COST EUSPEC Workshop and School "Xtram17 - XUV time resolved advanced methods" : experiments and ab-initio modeling
23/08/2017 → 28/08/2017
Erice, Italy
Activity: Talks and presentations › Conference presentations

25th Colloquium on High Resolution Molecular Spectroscopy
Period: 20 Aug 2017 → 25 Aug 2017
René Wugt Larsen (Participant)
Department of Chemistry
Degree of recognition: International

Related event
25th Colloquium on High Resolution Molecular Spectroscopy
20/08/2017 → 26/08/2017
Helsinki, Finland
Activity: Attending an event › Participating in or organising a conference

Bacterial Electrocatalysis of K₄[Fe(CN)₆] Oxidation
Period: 17 Aug 2017 → 20 Aug 2017
Zhiyong Zheng (Invited speaker)
Department of Chemistry
NanoChemistry

Description
The Sixteenth International Symposium on Electroanalytical Chemistry (16th ISEAC)
Degree of recognition: International
Documents:
Tentative Program-0719
Links:
http://iseac2017.csp.escience.cn/dct/page/1

Related event
The Sixteenth International Symposium on Electroanalytical Chemistry
17/08/2016 → 20/08/2017
Changchun, China
Activity: Talks and presentations › Conference presentations

Petr Štěpánek
Start date: 14 Aug 2017 → 18 Aug 2017
Sonia Coriani (Host)
Department of Chemistry
Degree of recognition: International
Activity: Hosting a guest lecturer
dDNP as an emergent real time analytical method for catalytic reactions
Period: 4 Jul 2017
Peter Andreas Boeg (Guest lecturer)
Center for Hyperpolarization in Magnetic Resonance
Department of Chemistry
Centre for Catalysis and Sustainable Chemistry
Organic Chemistry
Documents:
Abstract_PANBO_Euromar 17

Related event
EUROMAR 2017
02/07/2017 → 06/07/2017
Warsaw, Poland
Activity: Talks and presentations › Conference presentations

Electrochemical Catalysis of Inorganic Complex K₄[Fe(CN)]₆ by Shewanella oneidensis MR-1
Period: 2 Jul 2017 → 5 Jul 2017
Zhiyong Zheng (Other)
Department of Chemistry
NanoChemistry

Description
The interaction between metal and bacteria is a universal and important biogeochemical process in environment. As a dissimilatory metal reduction bacteria, the electrochemical active bacteria Shewanella oneidensis MR-1 can transfer intracellular electrons to minerals. This ability is attributed to the redox proteins localized to the outer-membrane, for example, the MtJC, MtkB, MtRA and CymA. Here we investigate its electrochemical properties towards redox inorganic redox compounds. It shows strong electrocatalysis toward electrochemical oxidation of K₄[Fe(CN)]₆. As a redox molecule, K₄[Fe(CN)]₆ gives a pair of redox peaks on voltammetry on bare glassy carbon electrode (GCE), symmetric with ideal peak-peak separation of about 60 mV, indicating of a reversible one-electron transfer process (blue curve, Figure 1). Surprisingly, the presence of Shewanella oneidensis MR-
1 on GCE results an asymmetric redox peak, with almost disappearance of the cathodic peak and strengthen of the anodic peak, which is a typical catalysis feature of electrochemical oxidation.

Further experiments show that *Shewanella oneidensis* MR-1 does not give such electrocatalysis to redox compounds such as Ru[([NH₃]₆)Cl₃] and Resorufin. Systematic study on the selectivity and electrocatalysis mechanisms of *Shewanella oneidensis* MR-1 are under investigation. The ability of *Shewanella oneidensis* MR-1 to catalyze redox action of inorganic metal complex compounds will provide an insight on metal cycles in nature.

Links:
http://www.eicc-4.dk/home.html

**Related event**

**Forth EuCheMS Inorganic Chemistry Conference (EICC-4)**
Period: 2 Jul 2017 → 5 Jul 2017
Copenhagen, Denmark
Activity: Talks and presentations › Conference presentations

**Forth EuCheMS Inorganic Chemistry Conference (EICC-4)**
Period: 2 Jul 2017 → 5 Jul 2017
Ranran Wu (Participant)
Yong Xiao (Participant)
Hans Erik Malager Christensen (Participant)
Feng Zhao (Participant)
Jingdong Zhang (Participant)
Department of Chemistry
NanoChemistry
Organic Chemistry
Metalloprotein Chemistry and Engineering

**Description**
Electrochemical Catalysis of Inorganic Complex K₄[Fe(CN)₆] by *Shewanella oneidensis* MR-1

The interaction between metal and bacteria is a universal and important biogeochemical process in environment. As a dissimilatory metal reduction bacteria, the electrochemical active bacteria *Shewanella oneidensis* MR-1 can transfer intracellular electrons to minerals. This ability is attributed to the redox proteins localized to the outer-membrane, for example, the MtrC, MtrB, MtrA and CymA⁺. Here we investigate its electrochemical properties towards redox inorganic redox compounds. It shows strong electrocatalysis toward electrochemical oxidation of K₄[Fe(CN)₆]. As a redox molecule, K₄[Fe(CN)₆] gives a pair of redox peaks on voltammetry on bare glassy carbon electrode (GCE), symmetric with ideal peak-peak separation of about 60 mV, indicating of a reversible one-electron transfer process (blue curve, Figure 1). Surprisingly, the presence of *Shewanella oneidensis* MR-1 on GCE results an asymmetric redox peak, with almost disappearance of the cathodic peak and strengthen of the anodic peak, which is a typical catalysis feature of electrochemical oxidation.

Further experiments show that *Shewanella oneidensis* MR-1 does not give such electrocatalysis to redox compounds such as Ru[([NH₃]₆)Cl₃] and Resorufin. Systematic study on the selectivity and electrocatalysis mechanisms of *Shewanella oneidensis* MR-1 are under investigation. The ability of *Shewanella oneidensis* MR-1 to catalyze redox action of inorganic metal complex compounds will provide an insight on metal cycles in nature.

Links:
http://www.eicc-4.dk/home.html

**Related event**

**Forth EuCheMS Inorganic Chemistry Conference (EICC-4)**
Period: 2 Jul 2017 → 5 Jul 2017
Copenhagen, Denmark
Activity: Attending an event › Participating in or organising a conference

**University of Southern Denmark (External organisation)**
Period: 30 Jun 2017
Susanne Mossin (Member)
Center for Hyperpolarization in Magnetic Resonance
Department of Chemistry
Centre for Catalysis and Sustainable Chemistry
Organic Chemistry

**Description**
Opponent at PhD defense

**Related external organisation**
University of Southern Denmark
Odense, Denmark
Activity: Membership › Membership in review committee

**Federica Frati**
Start date: 28 Jun 2017 → 7 Jul 2017
Sonia Coriani (Host)
Department of Chemistry
Degree of recognition: International
Activity: Hosting a guest lecturer

**Invited talk**
Period: 22 Jun 2017
Sonia Coriani (Invited speaker)
Department of Chemistry

**Related event**
New Frontiers in Electron Correlation
20/06/2017 → 24/06/2017
Telluride, United States
Activity: Talks and presentations › Conference presentations

**New Frontiers in Electron Correlation**
Period: 20 Jun 2017 → 24 Jun 2017
Sonia Coriani (Participant)
Department of Chemistry
Degree of recognition: International

**Related event**
New Frontiers in Electron Correlation
20/06/2017 → 24/06/2017
Telluride, United States
Activity: Attending an event › Participating in or organising a conference

**Lund University (External organisation)**
Period: 15 Jun 2017
Susanne Mossin (Chairman)
Center for Hyperpolarization in Magnetic Resonance
Department of Chemistry
Centre for Catalysis and Sustainable Chemistry
Organic Chemistry

**Description**
Opponent at PhD defense

Related external organisation

Lund University
Lund, Sweden
Activity: Membership › Membership in review committee

9th International Conference on Advanced Vibrational Spectroscopy
Period: 11 Jun 2017 → 17 Jun 2017
René Wugt Larsen (Participant)

Department of Chemistry
Degree of recognition: International
Links:
http://www.icavs.org/

Related event

9th International Conference on Advanced Vibrational Spectroscopy
11/06/2017 → 17/06/2017
Victoria, Canada
Activity: Attending an event › Participating in or organising a conference

Ultrafast electronic and nuclear dynamics in photo-excited transition-metal complexes
Period: 18 Apr 2017 → 21 Apr 2017
Klaus Braagaard Møller (Invited speaker)

Department of Chemistry

Description
CMST COST Action CM1405
Degree of recognition: International

Related event

International Workshop on Molecular Quantum Dynamics and Kinetics
18/04/2017 → 21/04/2017
Zürich, Switzerland
Activity: Talks and presentations › Conference presentations

International Conference: Molecular Properties and Computational Spectroscopy - from Esoteric Effects to Novel Probing Tools
Period: 10 Apr 2017 → 12 Apr 2017
Sonia Coriani (Organizer)

Department of Chemistry
Degree of recognition: International
Links:
http://mpcs17.pi.ipcf.cnr.it/ (Conference website)

Related event

International Conference: Molecular Properties and Computational Spectroscopy - from Esoteric Effects to Novel Probing Tools
09/04/2017 → 12/04/2017
Pisa, Italy
Activity: Attending an event › Participating in or organising a conference

Reviewer for FWO, Belgian Independent Research Council (External organisation)
Period: 9 Apr 2017
Susanne Mossin (Participant)
Center for Hyperpolarization in Magnetic Resonance
Department of Chemistry
Centre for Catalysis and Sustainable Chemistry
Organic Chemistry

Description
Reviewer for FWO, Belgian Independent Research Council
Degree of recognition: International

Related external organisation
Reviewer for FWO, Belgian Independent Research Council
Activity: Membership › Membership in review committee

Coupled Cluster Strategies for Core Spectroscopies of Ground and Excited States
Period: 24 Feb 2017
Sonia Coriani (Keynote speaker)
Department of Chemistry
Degree of recognition: International

Related event
The 57th Sanibel Meeting: The Theory Meeting for Theoreticians
19/02/2017 → 24/02/2017
St. St. Simons Island, GA, United States
Activity: Talks and presentations › Conference presentations

The 57th Sanibel Meeting
Period: 19 Feb 2017 → 24 Feb 2017
Sonia Coriani (Participant)
Department of Chemistry
Degree of recognition: International
Links:

Related event
The 57th Sanibel Meeting: The Theory Meeting for Theoreticians
19/02/2017 → 24/02/2017
St. St. Simons Island, GA, United States
Activity: Attending an event › Participating in or organising a conference

Single center reactivity of Cu(II) sites in copper substituted CHA zeolite followed by in-situ electron paramagnetic resonance spectroscopy
Period: 18 Nov 2016
Susanne Mossin (Speaker)
Center for Hyperpolarization in Magnetic Resonance
Department of Chemistry
Centre for Catalysis and Sustainable Chemistry
Organic Chemistry
Documents:
Mossin_aiche_2016

Related event
2016 AIChE Annual Meeting
Molecules in motion observed with X-rays
Klaus Braagaard Møller (Invited speaker)
Department of Chemistry

Description
CMST COST Action CM1405

Related event

2nd MOLIM General Meeting
10/10/2016 → 12/10/2016
Dubrovnik, Croatia
Activity: Talks and presentations › Conference presentations

Single center reactivity of Cu(II) sites in copper substituted CHA zeolite followed by in-situ electron paramagnetic resonance spectroscopy
Period: 28 Sep 2016
Susanne Mossin (Invited speaker)
Center for Hyperpolarization in Magnetic Resonance
Department of Chemistry
Centre for Catalysis and Sustainable Chemistry
Organic Chemistry

Related event

Organic/inorganic meeting LU/KU/DTU 2016
28/09/2016 → …
Lund, Sweden
Activity: Talks and presentations › Conference presentations

The Electrochemical Society (External organisation)
Period: Aug 2016
Arnab Halder (Participant)
Department of Chemistry
NanoChemistry
Organic Chemistry

Related external organisation

The Electrochemical Society
United States
Activity: Membership › Membership of research networks or expert groups

67th Annual Meeting of the International Society of Electrochemistry
Arnab Halder (Participant)
Department of Chemistry
NanoChemistry
Organic Chemistry
Related event

67th Annual Meeting of the International Society of Electrochemistry: Electrochemistry: from Sense to Sustainability
21/08/2016 → 26/08/2016
The Hague, Netherlands
Activity: Attending an event › Participating in or organising a conference

Reviewer for FWO, Belgian Independent Research Council (External organisation)
Period: 1 Jul 2016
Susanne Mossin (Participant)
Centre for Catalysis and Sustainable Chemistry
Department of Chemistry
Center for Hyperpolarization in Magnetic Resonance
Degree of recognition: International

Reviewer for FWO, Belgian Independent Research Council
Activity: Membership › Membership in review committee

18th International Zeolite Conference
Period: 23 Jun 2016
Søren Tolborg (Speaker)
Department of Chemistry
Organic Chemistry
Description
Oral contribution on the topic of "Shape-selectivity in Biomass Conversion: Zeotype-catalyzed Formation of C4 Sugars"
Conference participation and oral contribution
Documents:
Shape-selectivity in Biomass Conversion: Zeotype-catalyzed Formation of C4 Sugars

Related event

18th International Zeolite Conference: Zeolites for a Sustainable World
19/06/2016 → 24/06/2016
Rio de Janeiro, Brazil
Activity: Talks and presentations › Conference presentations

Single center reactivity of Cu(II) sites in Cu-CHA followed by in-situ EPR
Period: 15 Jun 2016
Susanne Mossin (Speaker)
Centre for Catalysis and Sustainable Chemistry
Department of Chemistry
Center for Hyperpolarization in Magnetic Resonance
Documents:
Mossin_nsc_2016

Related event

17th Nordic Symposium on Catalysis 2016: Surface science and catalysis for sustainable development and the use of large scale facilities for catalysis research
14/06/2016 → 16/06/2016
Lund, Sweden
Activity: Talks and presentations › Conference presentations
Incorporation of gold into zeolite silicalite-1 using pressure assisted impregnation and reduction method
Period: 9 Jun 2016
Agata Gallas-Hulin (Speaker)
Department of Chemistry
Centre for Catalysis and Sustainable Chemistry
Organic Chemistry

Related event
Annual Meeting of Danish Chemical Society 2016
09/06/2016 → 09/06/2016
Odense, Denmark
Activity: Talks and presentations › Conference presentations

Biosensors 2016
Period: 25 May 2016 → 27 May 2016
Arnab Halder (Participant)
Department of Chemistry
NanoChemistry
Organic Chemistry

Description
Electroactive polymer functionalized graphene nanocomposites as a biosensing platform

Related event
Biosensors 2016: 26th Anniversary World Congress on Biosensors
25/05/2016 → 27/05/2016
Gothenburg, Sweden
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

AFM Workshop: Latest Developments in SPM
Period: 16 Mar 2016
Arnab Halder (Participant)
Department of Chemistry
NanoChemistry
Organic Chemistry

Description
AFM Workshop: Latest Developments in SPM

Related event
AFM Workshop: Latest Developments in SPM
17/03/2016 → …
Kgs. Lyngby, Denmark
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Is more better?: Studies on the expansion from conventional mononuclear organometallic compounds to polynuclear cluster complexes and the resulting impact on reactivity will be presented.
Period: 24 Feb 2016
Martin Nielsen (Lecturer)
Department of Chemistry
Seminar at Leibniz-Institute for Catalysis
24/02/2016 → 24/02/2016
Rostock, Germany
Activity: Talks and presentations › Conference presentations

A consistent reaction mechanism for the selective catalytic reduction of NO with NH₃
Period: 2015
Susanne Mossin (Speaker)
Department of Chemistry
Centre for Catalysis and Sustainable Chemistry
Organic Chemistry

Bioelectrochemical society (External organisation)
Period: 2015
Arnab Halder (Participant)
Department of Chemistry
NanoChemistry
Organic Chemistry
Degree of recognition: International

Chemistry of the active metal center in the selective catalytic reduction of NO by NH₃
Period: 2015
Susanne Mossin (Speaker)
Department of Chemistry
Centre for Catalysis and Sustainable Chemistry
Organic Chemistry
Documents:
EuropaCatLongAbstract_Mossin

Bioelectrochemical society
Activity: Membership › Membership of research networks or expert groups

12th European Congress on Catalysis: Catalysis: Balancing the Use of Fossil and Renewable Resources
30/08/2015 → 05/09/2015
Kazan, Russian Federation
Activity: Talks and presentations › Conference presentations

**International Society of Electrochemistry (External organisation)**
Period: 2015
Arnab Halder (Participant)

NanoChemistry
Organic Chemistry

Department of Chemistry
Degree of recognition: International

**Related external organisation**
**International Society of Electrochemistry**
Activity: Membership › Membership of research networks or expert groups

**The International Chemical Congress of Pacific Basin Societies 2015**
Period: 15 Dec 2015 → 20 Dec 2015
René Wugt Larsen (Participant)

Department of Chemistry

**Description**
The International Chemical Congress of Pacific Basin Societies 2015

**Related event**
**The International Chemical Congress of Pacific Basin Societies 2015**
15/12/2015 → 20/01/2016
Honolulu, United States
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

**How to convert light to chemical energy – the initial steps**
Period: 10 Dec 2015
Klaus Braagaard Møller (Invited speaker)

Department of Chemistry

**Related event**
**Physical Chemistry Seminar**
10/12/2015 → 10/12/2015
Copenhagen, Denmark
Activity: Talks and presentations › Conference presentations

**Board member (External organisation)**
Period: Nov 2015 → …
Susanne Mossin (Participant)

Center for Hyperpolarization in Magnetic Resonance
Centre for Catalysis and Sustainable Chemistry

**Description**
Body type: Danish Chemical Society

**Related external organisation**
**Board member**
Activity: Membership › Membership of committees, commissions, boards, councils, associations, organisations, or similar
**DTU Chemistry PhD School Symposium 2015**  
Period: 5 Nov 2015 → 6 Nov 2015  
Arnab Halder (Participant)  
Department of Chemistry  
NanoChemistry  
Organic Chemistry  

**Description**  
PhD symposium 2015, DTU Chemistry  

**Related event**  
DTU Chemistry PhD School Symposium 2015  
05/11/2015 → 05/11/2015  
Kgs. Lyngby, Denmark  
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.  

**DTU Chemistry PhD School Symposium 2015**  
Period: 5 Nov 2015 → 6 Nov 2015  
Nedjelko Šeselj (Participant)  
Department of Chemistry  
NanoChemistry  

**Related event**  
DTU Chemistry PhD School Symposium 2015  
05/11/2015 → 05/11/2015  
Kgs. Lyngby, Denmark  
Activity: Attending an event › Participating in or organising a conference  

**Gold encapsulation in zeolites**  
Period: 5 Nov 2015 → 6 Nov 2015  
Agata Gallas-Hulin (Speaker)  
Department of Chemistry  
Centre for Catalysis and Sustainable Chemistry  
Organic Chemistry  
Documents:  
Abstract  

**Related event**  
2015 PhD Symposium Department of Chemistry, Technical University of Denmark, Kgs. Lyngby, Denmark  
05/11/2015 → 06/11/2015  
Activity: Talks and presentations › Conference presentations  

**Shandong University**  
Christian Engelbrekt (Visiting researcher)  
Department of Chemistry  
NanoChemistry  

**Description**  
Electrochemical characterization of hybrid nanomaterials of copper oxide and graphene oxide and investigation of pseudo-capacitance  
Activity: Visiting an external institution › Visiting another research institution
Facile synthesis of starch-scaffolded bimetallic Au-Pt nanostructure and electrocatalysis
Period: 9 Oct 2015
Christian Engelbrekt (Speaker)
Department of Chemistry
NanoChemistry

Related event
The 66th Annual Meeting of the International Society of Electrochemistry
04/10/2015 → 09/10/2015
Taipei, Taiwan, Province of China
Activity: Talks and presentations › Conference presentations

12th European Congress on Catalysis
Period: 2 Sep 2015
Søren Tolborg (Speaker)
Department of Chemistry
Organic Chemistry

Description
Oral contribution on the topic of "New Insights in the Catalytic Conversion of Sugars with Sn-Beta"
Conference participation and oral contribution
Links:
http://www.europacat2015.com/ (Official homepage for the 12th European Congress on Catalysis)

Related event
12th European Congress on Catalysis: Catalysis: Balancing the Use of Fossil and Renewable Resources
30/08/2015 → 05/09/2015
Kazan, Russian Federation
Activity: Talks and presentations › Conference presentations

12th European Congress on Catalysis
Period: 30 Aug 2015 → 5 Sep 2015
Mayra Melián Rodríguez (Participant)
Department of Chemistry
Centre for Catalysis and Sustainable Chemistry
Organic Chemistry

Description
Catalytic oxidation of veratryl alcohol to veratraldehyde
Poster presentation
Documents:
Abstract
Poster

Related event
12th European Congress on Catalysis: Catalysis: Balancing the Use of Fossil and Renewable Resources
30/08/2015 → 05/09/2015
Kazan, Russian Federation
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.
eTEM investigation of gold nanoparticle formation in recrystallized zeolite silicalite-1
Period: 30 Aug 2015 → 4 Sep 2015
Agata Gallas-Hulin (Speaker)
Department of Chemistry
Centre for Catalysis and Sustainable Chemistry
Organic Chemistry
Documents:
Extended abstract

Related event
12th European Congress on Catalysis – EuropaCat-XI, Kazan, Russia
30/08/2015 → 04/09/2015
Activity: Talks and presentations › Conference presentations

MOLIM General Meeting
Klaus Braagaard Møller (Invited speaker)
Department of Chemistry
Description
Ultrafast molecular motion: experiment and simulation
CMST COST Action CM1405

Related event
1st MOLIM General Meeting
26/08/2015 → 29/08/2015
Paris, France
Activity: Talks and presentations › Conference presentations

Interactions of a Glucagon-like peptide 1 and a Glucagon-like peptide 1 analogue, liraglutide, with the endogenous receptor
Period: 25 Aug 2015
Tine Maja Frederiksen (Lecturer)
Department of Chemistry
Description
Presentation at the Annual meeting of the Swedish Chemical Society 'Theoretical Chemistry Section 2015 - Baltic Lights'
Documents:
TCS_2015_TM_Frederiksen_slides

Related event
Annual meeting of the Swedish Chemical Society 'Theoretical Chemistry Section 2015': Baltic Lights
25/08/2015 → 27/11/2015
Kalmar, Sweden
Activity: Talks and presentations › Conference presentations

A glucagon-like peptide 1 analogue and its interactions with the endogenous receptor
Period: 24 Aug 2015
Tine Maja Frederiksen (Lecturer)
Department of Chemistry
Documents:
TMMD_2015_TM_Frederiksen_slides

Related event
Synthesis of plant cell wall 1,5-α-L-oligoarabinofuranosides
Period: 19 Aug 2015
Mathilde Daugaard (Lecturer)
Department of Chemistry
Organic Chemistry

The SAMENS Method for Gold Nanostructure Syntheses: Green Synthesis and Electrocatalysis
Period: 14 Aug 2015
Christian Engelbrekt (Speaker)
Department of Chemistry
NanoChemistry

6th Symposium on Carbon and Related Nanomaterials
Arnab Halder (Participant)
NanoChemistry
Organic Chemistry
Department of Chemistry

6th Symposium on Carbon and Related Nanomaterials
Nedjeljko Seselj (Participant)
Department of Chemistry
NanoChemistry
Description
6th symposium on carbon and related nanomaterials in Copenhagen titled "Carbonhagen" held at 13th and 14th of August 2015.
Documents:
Development of graphene-supported Pt catalysts for fuel cells

Related event

6th Symposium on Carbon and Related Nanomaterials
13/08/2015 → 14/08/2015
Copenhagen, Denmark
Activity: Attending an event › Participating in or organising a conference

University of Copenhagen (External organisation)
Period: 11 Aug 2015
Susanne Mossin (Participant)
Department of Chemistry
Centre for Catalysis and Sustainable Chemistry
Organic Chemistry

Description
PhD committee member for Waqas Sethi, University of Copenhagen:
3d/4f metal complexes of phenolic oximes New binding sites on Anderson polyoxometalates Metal complexes of the new THAME ligand

Related external organisation

University of Copenhagen
Thorvaldsensvej 40, DK-1871 Frederiksberg C, Copenhagen, Denmark
Activity: Membership › Membership of committees, commissions, boards, councils, associations, organisations, or similar

COST EXIL 1206 (External organisation)
Period: Jul 2015 → Jun 2017
Susanne Mossin (Chairman)
Center for Hyperpolarization in Magnetic Resonance
Department of Chemistry
Centre for Catalysis and Sustainable Chemistry
Organic Chemistry

Description
Short term scientific missin manager in COST program Exchange on Ionic Liquids
Degree of recognition: International

Related external organisation

COST EXIL 1206
Activity: Membership › Membership of committees, commissions, boards, councils, associations, organisations, or similar

12th International Femtochemistry Conference
Period: 13 Jul 2015 → 17 Jul 2015
Klaus Braagaard Møller (Participant)
Department of Chemistry

Description
Poster: Direct Dynamics Simulations of Metal Complexes in Solution for Interpretation of XFEL Results

Related event
12th International Femtochemistry Conference
13/07/2015 → 17/07/2015
Hamburg, Germany
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

8th International Conference on Advanced Vibrational Spectroscopy
Period: 12 Jul 2015 → 17 Jul 2015
René Wugt Larsen (Participant)
Department of Chemistry

Related event

8th International Conference on Advanced Vibrational Spectroscopy
12/07/2015 → 17/07/2015
Vienna, Austria
Activity: Attending an event › Participating in or organising a conference

XXIII International Symposium on Bioelectrochemistry and Bioenergetics
Arnab Halder (Participant)
Department of Chemistry
NanoChemistry

Description
Student helper

Related event

XXIII International Symposium on Bioelectrochemistry and Bioenergetics
14/06/2015 → 18/06/2015
Malmö, Sweden
Activity: Attending an event › Participating in or organising a conference

Facile synthesis of starch-scaffolded bimetallic Au-Pt nanostructures and their catalytic properties
Period: 11 Jun 2015
Christian Engelbrekt (Speaker)
Department of Chemistry
NanoChemistry

Related event

The Danish Chemical Society - Annual Meeting 2015
11/06/2012 → …
Odense, Denmark
Activity: Talks and presentations › Conference presentations

23rd International Symposium on Glycoconjugates
Period: 16 May 2015
Mads Hartvig Clausen (Participant)
Department of Chemistry
Organic Chemistry

Description
CPH assay: high-throughput screening of endo-glycoside hydrolases using novel chromogenic polysaccharide substrates
Participation and poster presentation

Related event
23rd International Symposium on Glycoconjugates
15/09/2015 → 20/09/2015
Split, Croatia
Activity: Attending an event › Participating in or organising a conference

3rd International Symposium on Green Chemistry
Period: 7 May 2015
Søren Tolborg (Speaker)
Department of Chemistry
Organic Chemistry

Description
Flash communication on the topic of "Stannosilicates for Catalytic Conversion of Sugar: Alkali Ions Boost the Yield"

Conference participation and flash communication
Documents:
Stannosilicates for catalytic conversion of sugar: alkali ions boost the yield
Links:
http://www.isgc2015.com/program/whole-program.html,1,49,2,0,0 (Program for ISGC 2015)

Related event
3rd International Symposium on Green Chemistry: The world Scientific Congress on Green Chemistry
03/05/2015 → 07/05/2015
La Rochelle, France
Activity: Talks and presentations › Conference presentations

Chemical Biology of the Plant Cell Wall
Mads Hartvig Clausen (Invited speaker)
Department of Chemistry
Organic Chemistry

Related event
Nordic Chemical Biology Meeting
05/05/2015 → 06/05/2015
Stockholm, Sweden
Activity: Talks and presentations › Conference presentations

Anharmonicity in Medium-Sized Molecules and Clusters
Period: 26 Apr 2015 → 30 Apr 2015
René Wugt Larsen (Participant)
Department of Chemistry

Related event
Anharmonicity in Medium-Sized Molecules and Clusters
26/04/2015 → 30/04/2015
Madrid, Spain
Activity: Attending an event › Participating in or organising a conference

COST Action Lignoval
Period: 3 Feb 2015 → 4 Feb 2015
Mayra Melián Rodríguez (Participant)
Department of Chemistry
Centre for Catalysis and Sustainable Chemistry
Organic Chemistry

Description
Aerobic oxidation of b-O-4 lignin model compound with solid catalysts

Oral presentation
Documents:
Abstract

Related event
COST Action Meeting: 2nd MC Meeting & First Workshop
03/02/2015 → 04/02/2015
Belgrade, Serbia
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

XVII Annual Linz Winter Workshop
Period: 30 Jan 2015 → 2 Feb 2015
Nedjeljko Seselj (Participant)
Department of Chemistry
NanoChemistry

Description
The Linz Winter Workshop focuses on biological single-molecule research and nanoscience. It includes force and optical microscopy/spectroscopy techniques. In 2015, special sessions on nano-medicine, transmembrane transporters, nanopores, and high-speed atomic force microscopy was organized. It is the aim to provide a common platform for industry and academia.

Related event
XVII Annual Linz Winter Workshop: Advances in Single-Molecule Research for Biology and Nanoscience
30/01/2015 → 02/02/2015
Linz, Austria
Activity: Attending an event › Participating in or organising a conference

62nd Pacific Conference on Spectroscopy and Dynamics
Period: 29 Jan 2015 → 1 Feb 2015
Jonas Andersen (Participant)
Department of Chemistry

Related event
62nd Pacific Conference on Spectroscopy and Dynamics
29/01/2015 → 01/02/2015
Pacific Grove, CA, United States
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

62nd Pacific Conference on Spectroscopy and Dynamics
Period: 29 Jan 2015 → 2 Feb 2015
René Wugt Larsen (Participant)
Department of Chemistry

Related event
62nd Pacific Conference on Spectroscopy and Dynamics
29/01/2015 → 01/02/2015
Pacific Grove, CA, United States
Activity: Attending an event › Participating in or organising a conference
XVII Linz Winterworkshop. Advances in Single-Molecule Research for Biology & Nanoscience
Period: 27 Jan 2015 → 2 Feb 2015
Arnab Halder (Participant)
Department of Chemistry
NanoChemistry

Description
The Linz Winter Workshop was focused on biological single-molecule research and nanoscience, and include force and optical microscopy/spectroscopy techniques. This year, special sessions were on nano-medicine, transmembrane transporters, nanopores, and high-speed atomic force microscopy will be organized.

Related event
XVII Linz Winterworkshop. Advances in Single-Molecule Research for Biology & Nanoscience
27/01/2015 → 02/02/2016
Austria
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Dehydration of copper substituted zeolites: EPR studies of the in-situ generation of active sites for NH3-SCR deNOx catalysts
Period: 2014
Susanne Mossin (Lecturer)
Department of Chemistry
Centre for Catalysis and Sustainable Chemistry

Description
Foredrag

Related event
ACS
23/03/2014 → 27/03/2014
Dallas, United States
Activity: Talks and presentations › Conference presentations

DTU Chemistry PhD School Symposium 2014
Period: 2014
Arnab Halder (Participant)
Department of Chemistry
NanoChemistry
Organic Chemistry

Related event
DTU Chemistry PhD School Symposium 2014
20/11/2014 → 21/11/2014
Kgs. Lyngby, Denmark
Activity: Attending an event › Participating in or organising a conference

EPR of Cu-CHA: Identification and quantification of copper species present after dehydration
Period: 2014
Susanne Mossin (Lecturer)
Department of Chemistry
Centre for Catalysis and Sustainable Chemistry

Related event
16th Nordic Symposium on Catalysis 2014: From fundamentals to industrial application
15/06/2014 → 17/06/2014
Oslo, Norway
Activity: Talks and presentations › Conference presentations

DTU Chemistry PhD School Symposium 2014
Period: 20 Nov 2014 → 21 Nov 2014
Nedjelko Seselj (Participant)
Department of Chemistry
NanoChemistry
Documents:
Chemical Production of Graphene Catalysts for Electrochemical Energy Conversion

Related event
DTU Chemistry PhD School Symposium 2014
20/11/2014 → 21/11/2014
Kgs. Lyngby, Denmark
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Training analytical laboratories in Suriname: Research-based advice
Period: 1 Dec 2014 → 16 Nov 2014
Jens Andersen (Participant)
Department of Chemistry
Analytical Chemistry
Description
EU EDES-COLEACP project
Organizer
Activity: Other

Training analytical laboratories in Papua New Guinea: Research-based advice
Jens Andersen (Participant)
Department of Chemistry
Analytical Chemistry
Description
EU project/EDES-COLEACP
Organizer
Activity: Other

6th Conference of the Federation of European Zeolite Associations
Period: 10 Sep 2014
Søren Tolborg (Speaker)
Department of Chemistry
Organic Chemistry
Description
Poster workshop presentation on the topic of “New Insights into the Synthesis of Sn-Beta Catalyst”
Conference participation and poster workshop presentation
Documents:
New insights into the synthesis of Sn-Beta catalyst
Links:
http://events.dechema.de/events_media/FEZA2014_lecture_programme-p-6580.pdf (Program of the 6th FEZA conference)
Related event

**6th Conference of the Federation of European Zeolite Associations: Porous Systems: From Novel Materials to Sustainable Solutions**

08/09/2014 → 11/09/2014
Leipzig, Germany
Activity: Talks and presentations › Conference presentations

**XFEL Symposium**

Klaus Braagaard Møller (Invited speaker)
Department of Chemistry

**Description**

Dynamics of chemical bond formation – on the computer

**Related event**

**XFEL Symposium**

25/08/2014 → 27/08/2014
Sørup, Denmark
Activity: Talks and presentations › Conference presentations

**5th Symposium on Carbon Nanomaterials**

Arnab Halder (Participant)
Department of Chemistry
NanoChemistry
Organic Chemistry

**Related event**

**5th Symposium on Carbon Nanomaterials**

21/08/2014 → 22/08/2014
Copenhagen, Denmark
Activity: Attending an event › Participating in or organising a conference

**5th Symposium on Carbon Nanomaterials**

Nedjeljko Seselj (Participant)
Department of Chemistry
NanoChemistry

**Description**

5th Symposium on Carbon Nanomaterials is a two day symposium on graphene, carbon nanotubes, and other two-dimensional nanomaterials (e.g. boron-nitride, black phosphorene, molybdenum-disulfide and other TMDCs) jointly organised by Technical University of Denmark, University of Copenhagen and Århus University.

**Related event**

**5th Symposium on Carbon Nanomaterials**

21/08/2014 → 22/08/2014
Copenhagen, Denmark
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

**X-ray powder diffraction: A powerful tool for industrial protein production**

Christian Grundahl Frankær (Lecturer)
Department of Chemistry

X-ray Crystallography

**Related event**

**23rd Congress and General Assembly of the International Union of Crystallography**

05/08/2014 → 12/08/2014  
Montréal, Canada  

Activity: Talks and presentations › Conference presentations

**CO2 uptake in supported ionic liquid phase materials**

Helene Kolding (Lecturer)  
Department of Chemistry  
Centre for Catalysis and Sustainable Chemistry

**Related event**

**Conference on Molten Salts and Ionic Liquids**

06/07/2014 → 11/07/2014  
Tallin, Estonia

Activity: Talks and presentations › Conference presentations

**Aalborg University (External organisation)**

Period: Jun 2014  
Susanne Mossin (Participant)  
Department of Chemistry  
Centre for Catalysis and Sustainable Chemistry

**Description**

Medlem af Lektorbedømmelsesudvalg

**Related external organisation**

**Aalborg University**  
A.C. Meyers Vænge 15, 2450 Copenhagen SV, Aalborg, Denmark  

Activity: Membership › Membership in review committee

**2014 Chalmers Soft Matter Graduate Summer School**

Nedjeljko Seselj (Participant)  
Department of Chemistry  
NanoChemistry

**Description**

Chalmers PhD Graduate School "Chalmers Soft Matter Graduate School on Molecular Electronics and Molecular Switches" from the 23rd -28th June 2014, organized by Chalmers University of Technology, Gothenburg, Sweden. Topics of the Ph.D school covers single molecule devices, molecular switches, fabrication methods, graphene, molecular solar thermal, single molecule spin and theory.  
Documents:

2014 Chalmers Soft Matter Graduate Summer School "Molecular Electronics and Molecular Switches"

**Related event**

**2014 Chalmers Soft Matter Graduate Summer School: Molecular Electronics and Molecular Switches**

23/06/2014 → 28/06/2014  
Nösunds, Sweden

Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.
From Chemistry to Food and Energy
Martin Nielsen (Lecturer)
Department of Chemistry
Centre for Catalysis and Sustainable Chemistry
Organic Chemistry
Links:
http://esof2014.org/

Related event
ESOF2014 Copenhagen Euroscience Open Forum
21/06/2014 → 25/06/2014
Valby, Denmark
Activity: Talks and presentations › Conference presentations

From Chemistry to Food and Energy
Period: 19 Jun 2014 → 20 Jun 2014
Martin Nielsen (Lecturer)
Department of Chemistry
Centre for Catalysis and Sustainable Chemistry
Organic Chemistry
Links:

Related event
ESOF Marie Skłodowska-Curie actions Conference
19/06/2014 → 20/06/2014
Copenhagen, Denmark
Activity: Talks and presentations › Conference presentations

16th Nordic Symposium on Catalysis
Period: 15 Jun 2014 → 17 Jun 2014
Mayra Melián Rodríguez (Participant)
Department of Chemistry
Centre for Catalysis and Sustainable Chemistry
Organic Chemistry
Description
Heterogeneous catalysis on oxidation of lignin model compounds
Poster presentation
Documents:
Abstract
Poster

Related event
16th Nordic Symposium on Catalysis 2014: From fundamentals to industrial application
15/06/2014 → 17/06/2014
Oslo, Norway
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.
16th Nordic symposium on Catalysis, Oslo, Norway
Period: 15 Jun 2014 → 17 Jun 2014
Agata Gallas-Hulin (Participant)
Department of Chemistry
Centre for Catalysis and Sustainable Chemistry
Organic Chemistry
Description
Poster presentation
Documents:
Abstract

Related event
16th Nordic symposium on Catalysis, Oslo, Norway
15/06/2014 → 17/06/2014
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

CO₂ uptake in supported ionic liquid phase materials
Period: 15 Jun 2014 → 17 Jun 2014
Helene Kolding (Lecturer)
Department of Chemistry
Centre for Catalysis and Sustainable Chemistry

Related event
16th Nordic Symposium on Catalysis 2014: From fundamentals to industrial application
15/06/2014 → 17/06/2014
Oslo, Norway
Activity: Talks and presentations › Conference presentations

Molecules in Motion
Period: 10 Jun 2014 → 12 Jun 2014
Klaus Braagaard Møller (Invited speaker)
Department of Chemistry
Description
Ultrafast molecular motion: theory and experiment

Related event
Molecules in Motion
10/06/2014 → 12/06/2014
Dragør, Denmark
Activity: Talks and presentations › Conference presentations

Summer School on Catalysis of Biomass
Period: 8 Jun 2014 → 11 Jun 2014
Mayra Melián Rodríguez (Participant)
Department of Chemistry
Centre for Catalysis and Sustainable Chemistry
Organic Chemistry
Description
Lignin valorization using heterogeneous catalytic oxidation
Poster presentation
Documents:
Abstract
Poster

Related event

Summer School on Catalysis of Biomass: CASCATBEL
08/06/2014 → 11/06/2014
Liblice, Czech Republic
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Aerobic oxidation of allyl alcohol in ambient conditions using supported nanoparticle gold catalyst
Period: 1 Jun 2014 → 6 Jun 2014
Agata Gallas-Hulin (Speaker)
Department of Chemistry
Centre for Catalysis and Sustainable Chemistry
Organic Chemistry
Documents:
Extended abstract

Related event

7th Tokyo Conference on Advanced Catalysis Science and technology
01/06/2014 → 06/06/2014
Kyoto, Japan
Activity: Talks and presentations › Conference presentations

Quantum and classical complexity
Period: 5 May 2014 → 7 May 2014
Klaus Braagaard Møller (Invited speaker)
Department of Chemistry
Description
Chemical dynamics in complex systems.

Related event

Quantum and classical complexity: From atoms to biosystems
05/05/2014 → 07/05/2014
Bad Homburg, Germany
Activity: Talks and presentations › Conference presentations

4th International Congress in Green Process Engineering
Period: 7 Apr 2014 → 10 Apr 2014
Mayra Melián Rodríguez (Participant)
Department of Chemistry
Centre for Catalysis and Sustainable Chemistry
Organic Chemistry
Description
Lignin valorization by heterogeneous catalytic oxidation
Poster presentation
Documents:
Abstract

Related event
4th International Congress in Green Process Engineering  
07/04/2014 → 10/04/2014  
Sevilla, Spain  
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

**Member of Danish censor corps of Chemistry (External organisation)**  
Period: 1 Apr 2014 → 30 Mar 2018  
Jens Andersen (Participant)  
Department of Chemistry  
Analytical Chemistry  

**Description**  
Censor at university level.  
External censorship of bachelor projects, master projects and PhD projects.  
Body type: Governmental

**Related external organisation**  
**Member of Danish censor corps of Chemistry**  
Activity: Membership › Membership in review committee

**NanoSight User Meeting Copenhagen**  
Period: 1 Apr 2014  
Arnab Halder (Participant)  
Department of Chemistry  
NanoChemistry  
Organic Chemistry  

**Description**  
NanoSight User Meeting Copenhagen  

**Related event**  
**NanoSight User Meeting Copenhagen**  
01/04/2014 → …  
Greve, Denmark  
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

**CO2 uptake in supported ionic liquids phase materials**  
Helene Kolding (Lecturer)  
Department of Chemistry  
Centre for Catalysis and Sustainable Chemistry  

**Description**  
ENVR 161

**Related event**  
**247th ACS National Meeting: Chemistry & Materials for Energy**  
16/03/2014 → 20/03/2014  
Dallas, United States  
Activity: Talks and presentations › Conference presentations

**25th Austin Symposium on Molecular Structure and Dynamics at Dallas**  
Period: 1 Mar 2014 → 4 Mar 2014
Jonas Andersen (Participant)
Department of Chemistry
X-ray Crystallography

Description
25th Austin Symposium on Molecular Structure and Dynamics at Dallas.

Related event
25th Austin Symposium on Molecular Structure and Dynamics at Dallas
01/03/2014 → 04/03/2014
Dallas, Texas, United States
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

René Wugt Larsen (Participant)
Department of Chemistry

Related event
25th Austin Symposium on Molecular Structure and Dynamics at Dallas
Period: 1 Mar 2014 → 4 Mar 2014
Dallas, Texas, United States
Activity: Attending an event › Participating in or organising a conference

Metrohm Autolab NOVA Software seminar
Period: 27 Feb 2014
Arnab Halder (Participant)
Department of Chemistry
NanoChemistry
Organic Chemistry

Description
Metrohm Autolab NOVA Software seminar

Related event
Metrohm Autolab NOVA Software seminar
27/02/2014 → …
Glostrup, Denmark
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Towards a hydrogen-based economy: Low-temperature hydrogen production from aqueous methanol
Period: 2013
Martin Nielsen (Lecturer)
Department of Chemistry
Centre for Catalysis and Sustainable Chemistry
Organic Chemistry

Description
It is today well known that we all have an interest in replacing fossil fuels as energy source with more renewable sources. In order to develop a sustainable energy system that can compete with the fossil-based system, renewable hydrogen production has been suggested as the central means of accessing chemically stored energy. This has been termed hydrogen economy. In order to make an energy system based on hydrogen realistic, a method for efficient and safe transport of the hydrogen needs to be developed. For this, methanol is a promising candidate as a hydrogen-rich and easily transportable material. The idea is that methanol is produced via e.g. hydrogenation of carbon dioxide, thereby storing the hydrogen. This is part of a bigger term, the methanol economy. One major obstacle for this type of the
methanol economy to become viable is the release of the hydrogen, which has to be done at relatively mild conditions in order not to use more energy during this process than the resulting hydrogen will provide. Here, we show our contribution to this endeavour. We show the first reported homogeneous catalytic system for the production of hydrogen and carbon dioxide from an aqueous methanol solution. We can reach the same gaseous hydrogen/carbon dioxide of 3:1 as is characteristic of methanol reforming, a process which has otherwise exclusively been carried out by heterogeneous catalysis. In addition, our system is mild compared to the heterogeneous system with working temperatures <100 °C. We also show the robustness of the system by letting it perform for more than three weeks. The maximum turnover frequency (TOFmax) is 4700 h⁻¹ and the turnover number exceeds 350000. Reference: Low-temperature aqueous-phase methanol dehydrogenation to hydrogen and carbon dioxide, Nielsen, M.; Alberico, E.; Baumann, W.; Drexler, H.-J.; Junge, H.; Gladiali, S.; Beller, M. Nature, 2013 , 495, 85.

Related event

246th ACS National Meeting & Exposition
08/09/2013 → 12/09/2013
Indianapolis, Indiana, United States
Activity: Talks and presentations › Conference presentations

Towards sustainable energy: Hydrogen production from biomass
Period: 2013
Martin Nielsen (Lecturer)
Department of Chemistry
Centre for Catalysis and Sustainable Chemistry
Organic Chemistry

Description
There is interest in developing alternative energy networks to the current fossil-based system. Some of the more promising emerging alternatives use hydrogen as the energy carrier. Hence, for these method to become viable we need to develop cost-efficient and sustainable techniques for the production of hydrogen.

Here, we present our latest findings in hydrogen production from biomass rich in alcohol units by use of homogeneous catalysis and relatively mild conditions. The biomass substrates include e.g. bioethanol, glycerol, and carbohydrates. Activities with unprecedented turnovers per hour will be presented.

On top of producing hydrogen from organic substances, it is theoretically possible to concurrently form valuable organic product. A single practical example of this will be presented as well.

References (only those with already assigned DOI numbers by submission date are included):

Related event

246th ACS National Meeting & Exposition
08/09/2013 → 12/09/2013
Indianapolis, Indiana, United States
Activity: Talks and presentations › Conference presentations

Towards sustainable energy using homogeneous catalysis
Period: 2013
Martin Nielsen (Lecturer)
Department of Chemistry
Centre for Catalysis and Sustainable Chemistry
Organic Chemistry

Related event

Kemisk Forening årsmøde
06/06/2013 → 06/06/2013
Odense, Denmark
**Training Analytical Laboratories in Jamaica: ICP-MS determination of heavy metals in food products**  
**Period:** 9 Dec 2013 → 20 Dec 2013  
**Jens Andersen (Participant)**  
**Department of Chemistry**  
**Analytical Chemistry**  

**Description**  
Quality assurance and preparation for accreditation of laboratory for analysis of heavy metals in samples of food products according to regulations of the European Union.

Planning of training and execution of training for analysis with inductively-coupled plasma mass spectrometry (ICP-MS) of heavy metals and semimetals arsenic, iron, zink, cadmium, lead and mercury in food products of Jamaica.

EDES-COLEACP of the European Comission

**Related external organisation**  
**Technical University of Denmark**  
Kgs. Lyngby, Denmark

**Winter School in Theoretical Chemistry**  
**Period:** 9 Dec 2013 → 12 Dec 2013  
**Jonas Andersen (Participant)**  
**Department of Chemistry**  
**X-ray Crystallography**

**Related event**  
**Winter School in Theoretical Chemistry**  
09/12/2013 → 12/12/2013  
Helsinki, Finland

**CO2 uptake in supported ionic liquid phase (SILP) materials**  
**Period:** 11 Nov 2013 → 12 Nov 2013  
**Helene Kolding (Lecturer)**  
**Department of Chemistry**  
**Centre for Catalysis and Sustainable Chemistry**

**Related event**  
**DTU Chemistry PhD Symposium**  
Sore, Denmark

**MS Öresund**  
**Period:** 24 Sep 2013  
**Kasper Skov (Speaker)**  
**Department of Systems Biology**  
**Department of Chemistry**  
**National Food Institute**
Division of Food Chemistry

**Description**
Short talk about my project EDC effects on the rat plasma metabolome.

Presentation at MS Øresund.

**Related event**
**Mass Spectrometry Users Meeting 2013**
24/09/2013 → 24/09/2013
Lund, Sweden
Activity: Talks and presentations › Talks and presentations in private or public companies and organisations

2nd International Congress on Catalysis for Biorefineries
Period: 22 Sep 2013 → 28 Sep 2013
Mayra Melián Rodríguez (Participant)
Department of Chemistry
Centre for Catalysis and Sustainable Chemistry
Organic Chemistry

**Description**
Conversion of lignin into chemicals with heterogeneous catalysis. Current and future technologies

Poster Presentation
Award: Poster Prize
Documents:
Abstract
Poster

**Related event**
2nd International Congress on Catalysis for Biorefineries
22/09/2013 → 28/09/2015
Dalian, China
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Training Analytical Laboratories in Kenya – Heavy Metals in Food Products: EDES 100003/CSM/DTU/028/KEN Ref 1200
Period: 8 Sep 2013 → 20 Sep 2013
Jens Andersen (Guest lecturer)
Department of Chemistry
Analytical Chemistry

**Description**
Science-based services. Training laboratory staff in determination of heavy metals in food products by using FAAS and GFAAS and preparing for accreditation

Organised by DTU Food. Planning of course and lecturing at KEPHIS

Participants also from Kenyan Bureau of Standards (KEBS)
Links:
http://edes.coleacp.org/en (Responsible organiser)
http://www.food.dtu.dk/ (Local organising for expert)

**Related external organisation**
Kenya Plant Health Inspectorate Services (KEPHIS)
Nairobi, Kenya
Activity: Talks and presentations › Guest lectures, external teaching and course activities at other universities
11th European Congress on Catalysis  
Period: 1 Sep 2013 → 6 Sep 2013  
Helene Kolding (Participant)  
Department of Chemistry  
Centre for Catalysis and Sustainable Chemistry  
Related event

11th European Congress on Catalysis  
01/09/2013 → 06/09/2013  
Lyon, France  
Activity: Attending an event › Participating in or organising a conference

11th European Congress on Catalysis  
Period: 1 Sep 2013 → 6 Sep 2013  
Mayra Melián Rodríguez (Participant)  
Department of Chemistry  
Centre for Catalysis and Sustainable Chemistry  
Organic Chemistry  
Related event

11th European Congress on Catalysis  
Period: 1 Sep 2013 → 6 Sep 2013  
Mayra Melián Rodríguez (Participant)  
Department of Chemistry  
Centre for Catalysis and Sustainable Chemistry  
Organic Chemistry  
Related event

Shanghai University  
Period: 1 Sep 2013 → 27 Oct 2013  
Christian Engelbrekt (Visiting researcher)  
Department of Chemistry  
NanoChemistry  
Description

Synthesis of gold nanoparticle-titanium dioxide composites and testing for photoelectrocatalytic degradation of organic molecules  
Visiting scholar  
Activity: Visiting an external institution › Visiting another research institution

Pitfalls in Teaching QA/QC  
Period: 26 Aug 2013  
Jens Andersen (Invited speaker)  
Department of Chemistry  
Analytical Chemistry  
Description

Particular attention should be given to the concepts of precision, accuracy, rejection of outliers, standard addition, limit of detection (LOD), lower-limit of analysis (LLA) and upper-limit of analysis (ULA) where pitfalls in data management may lead to major errors in analysis. Several schools of QA promote different recommendations which may lead to inconsistent results and decisions. Therefore are required further investigations into the origin of significant deviations, which are observed for average values and uncertainties of e.g. inter-laboratory comparisons. Tentative correlation between results of inter-laboratory comparisons and intra-laboratory comparisons is discussed. Quality assurance (QA) and quality control (QC) are important tools of analytical chemistry, and several topics and concepts within statistics are required in order to perform reliable data management. Linear regression is applied to operational calibrations of analytical apparatus, and straight lines with correlation coefficients, most frequently, close to one are published in analytical chemistry. Calculation
of regression line is a straightforward mathematical procedure, but the associated calculation of uncertainty needs more attention. Conversely, the standard-addition method (SAM) seems uncomplicated but there are a number of pitfalls that need be considered before reliable results may be produced. Teaching in principles is important to students and the vast majority of time in the lecture theatre is spent on understanding of principles of chemical mechanisms. However when principles are supposed to be implemented in practical examples, that are important to innovation and entrepreneurship, then occupies estimation of uncertainty a key position; uncertainties lead the way to genuine results of science. Since the evaluation of statistical data has not yet arrived at a standardized stage of utilization in science, are treated advantages and drawbacks with respect to different methodologies of QA and QC. A profound understanding of uncertainties of linear regression is presented, which includes comparison of different methodologies and aiming at simplicity in data interpretation.

Invited speaker chaired by Reiner Salzer

Related event

**Euroanalysis XVII: Analytical Chemistry for Human Well-being and Sustainable Development**
25/08/2013 → 29/08/2013
Warsaw, Poland
Activity: Talks and presentations › Conference presentations

**Dynamic Approach to the Study of Green Nanoparticle Formation**
Period: 19 Aug 2013
Christian Engelbrekt (Speaker)
Department of Chemistry
NanoChemistry

**Description**
Authors: Christian ENGELBREKT, Jens ULSTRUP, Jingdong ZHANG

**Related event**

**14th International Symposium on Electroanalytical Chemistry**
17/08/2013 → 20/08/2013
Changchun, China
Activity: Talks and presentations › Conference presentations

**Shandong University**
Period: 15 Aug 2013 → 31 Aug 2013
Christian Engelbrekt (Visiting researcher)
Department of Chemistry
NanoChemistry

**Description**
Green synthesis of supported PdPt alloy nanoparticles and testing in direct methanol and formic acid fuel cells

**Visiting scholar**
Activity: Visiting an external institution › Visiting another research institution

**The Copenhagen Conference on Femtochemistry**
Period: 7 Jul 2013 → 12 Jul 2013
Klaus Braagaard Møller (Organizer)
Department of Chemistry
Physical and Biophysical Chemistry

**Related event**

**The Copenhagen Conference on Femtochemistry**
07/07/2013 → 12/07/2013
Kgs. Lyngby, Denmark
21st International Conference on Laser Spectroscopy  
Period: 9 Jun 2013 → 14 Jun 2013  
René Wugt Larsen (Participant)  
Department of Chemistry

Related event

21st International Conference on Laser Spectroscopy  
09/06/2013 → 15/06/2013  
Berkeley, United States  
Activity: Attending an event › Participating in or organising a conference

5th Conference on Ionic Liquids  
Period: 21 Apr 2013 → 25 Apr 2014  
Helene Kolding (Participant)  
Department of Chemistry  
Centre for Catalysis and Sustainable Chemistry

Related event

5th Conference on Ionic Liquids  
21/04/2013 → 25/04/2013  
Vilamoura, Portugal  
Activity: Attending an event › Participating in or organising a conference

Chemical Dynamics and Spectroscopy  
Period: 8 Apr 2013 → 12 Apr 2013  
Klaus Braagaard Møller (Invited speaker)  
Department of Chemistry  
Physical and Biophysical Chemistry

Related event

Rome School on Open Systems and the Quantum-Classical Boundary  
08/04/2013 → 12/04/2013  
Rome, Italy  
Activity: Talks and presentations › Conference presentations

A Mononuclear Fe(III) Single Molecule Magnet with a 3/2↔5/2 Spin Crossover  
Period: 2012 → …  
Susanne Mossin (Lecturer)  
Department of Chemistry

Related event

243rd ACS National Meeting  
25/03/2012 → 29/03/2012  
San Diego, CA, United States  
Activity: Talks and presentations › Conference presentations

Winter School for Theoretical Chemistry and Spectroscopy  
Period: 10 Dec 2012 → 14 Dec 2012  
Jonas Andersen (Participant)  
Department of Chemistry
X-ray Crystallography

Related event

Winter School for Theoretical Chemistry and Spectroscopy
10/12/2012 → 14/12/2012
Han-Sur-Lesse, Belgium
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Pooled calibrations and retention of outliers improve chemical analysis
Period: 21 Sep 2012
Jens Andersen (Speaker)
Department of Chemistry
Analytical Chemistry
Degree of recognition: International

Related event

1st International Conference on Analytical Chemistry: Analytical Chemistry for a better life
18/09/2012 → 21/09/2012
Targoviste, Romania
Activity: Talks and presentations › Conference presentations

Fe(III) Single Molecule Magnet with a 3/2↔5/2 Spin Crossover
Period: 10 Sep 2012
Susanne Mossin (Lecturer)
Department of Chemistry

Related event

40th International Conference on Coordination Chemistry
09/09/2012 → 13/09/2012
Valencia, Spain
Activity: Talks and presentations › Conference presentations

Ph.D. Evaluation Committee (External organisation)
Period: 11 Jun 2012 → 31 Aug 2012
Jens Andersen (Participant)
Department of Chemistry
Analytical Chemistry

Description
Ph.D. defense

University of Tartu, Estonia

Body type: University
Degree of recognition: International

Related external organisation

Ph.D. Evaluation Committee
Activity: Membership › Membership of committees, commissions, boards, councils, associations, organisations, or similar

Shanghai Institute of Applied Physics
Christian Engelbrekt (Visiting researcher)
Department of Chemistry
NanoChemistry

**Description**
Characterization of synthesized copper minerals by synchrotron techniques at the SSRF

**Visiting scholar**
Activity: Visiting an external institution › Visiting another research institution

**SAMENS: A Green Approach to the Synthesis of Classical and New Metallic Nanostructures**
Period: 17 Jan 2012
Christian Engelbrekt (Speaker)
Department of Chemistry
NanoChemistry
 Documents: Capture

**Related event**

**DTU Nanoparticle Network Workshop**
17/01/2012 → …
Lyngby, Denmark
Activity: Talks and presentations › Conference presentations

**Electrocatalysis of interfacial bioelectrochemical electron transfer processes at the single-molecule level**
Period: 14 Sep 2011 → 17 Sep 2011
Jingdong Zhang (Keynote speaker)
Department of Chemistry
NanoChemistry

**Description**
The structure, two-dimensional surface organization, and electron transfer (ET) function of biological macromolecules and biomimetic molecules on solid surfaces can now be addressed at a degree of detail that reaches the level of the single molecule. ET metalloproteins such as blue copper, heme, and iron-sulfur proteins have thus become new target molecules for single-molecule electrochemical surface science. Redox molecules such as these are "smart" molecules in the sense that they can be brought to "do" something in their natural aqueous biological buffer environment. Scanning tunnelling and atomic force microscopy in aqueous biological media supported by theoretical frames are core approaches in these new areas. We overview here some new recent efforts in electrocatalysis of redox metalloenzymes and biomimetic metalloenzyme models also brought to the single-molecule level. Structures and enzyme mechanisms of these large and composite biomolecular entities offer new challenges. We shall address: • Binding modes of molecular linkers on electrochemical Au(111)-electrode surfaces. • A biomimetic metalloenzyme unit – the [Mo3S4]3+/4+ cluster. • Interfacial bioelectrochemical catalysis by "normal" and "green" gold nanoparticles. • Single-molecule bioelectrocatalysis - multi-copper nitrite reductase and laccases.

Documents:
alicante.pdf

**Related event**

Electrocatalysis of interfacial bioelectrochemical electron transfer processes at the single-molecule level: Invited keynote/tutorial communication, FP7 Marie Curie Training Network Programme ELCAT, University of Alicante
14/09/2011 → 17/09/2011
Alicante, Spain
Activity: Talks and presentations › Conference presentations

**Electrocatalysis of interfacial bioelectrochemical electron transfer processes at the single-molecule level**
Period: 14 Sep 2011 → 17 Sep 2011
Palle Skovhus Jensen (Keynote speaker)
Department of Chemistry
NanoChemistry
The structure, two-dimensional surface organization, and electron transfer (ET) function of biological macromolecules and biomimetic molecules on solid surfaces can now be addressed at a degree of detail that reaches the level of the single molecule. ET metalloproteins such as blue copper, heme, and iron-sulfur proteins have thus become new target molecules for single-molecule electrochemical surface science. Redox molecules such as these are "smart" molecules in the sense that they can be brought to "do" something in their natural aqueous biological buffer environment. Scanning tunnelling and atomic force microscopy in aqueous biological media supported by theoretical frames are core approaches in these new areas. We overview here some new recent efforts in electrocatalysis of redox metalloenzymes and biomimetic metalloenzyme models also brought to the single-molecule level. Structures and enzyme mechanisms of these large and composite biomolecular entities offer new challenges. We shall address: • Binding modes of molecular linkers on electrochemical Au(111)-electrode surfaces. • A biomimetic metalloenzyme unit – the [Mo3S4]3+/4+ cluster. • Interfacial bioelectrochemical catalysis by "normal" and "green" gold nanoparticles. • Single-molecule bioelectrocatalysis - multi-copper nitrite reductase and laccases.

Documents:
alicante.pdf

Related event

Electrocatalysis of interfacial bioelectrochemical electron transfer processes at the single-molecule level: Invited keynote/tutorial communication, FP7 Marie Curie Training Network Programme ELCAT, University of Alicante
14/09/2011 → 17/09/2011
Alicante, Spain
Activity: Talks and presentations › Conference presentations

Electrocatalysis of interfacial bioelectrochemical electron transfer processes at the single-molecule level
Period: 14 Sep 2011 → 17 Sep 2011
Qijin Chi (Keynote speaker)
Department of Chemistry
NanoChemistry

Description
The structure, two-dimensional surface organization, and electron transfer (ET) function of biological macromolecules and biomimetic molecules on solid surfaces can now be addressed at a degree of detail that reaches the level of the single molecule. ET metalloproteins such as blue copper, heme, and iron-sulfur proteins have thus become new target molecules for single-molecule electrochemical surface science. Redox molecules such as these are "smart" molecules in the sense that they can be brought to "do" something in their natural aqueous biological buffer environment. Scanning tunnelling and atomic force microscopy in aqueous biological media supported by theoretical frames are core approaches in these new areas. We overview here some new recent efforts in electrocatalysis of redox metalloenzymes and biomimetic metalloenzyme models also brought to the single-molecule level. Structures and enzyme mechanisms of these large and composite biomolecular entities offer new challenges. We shall address: • Binding modes of molecular linkers on electrochemical Au(111)-electrode surfaces. • A biomimetic metalloenzyme unit – the [Mo3S4]3+/4+ cluster. • Interfacial bioelectrochemical catalysis by "normal" and "green" gold nanoparticles. • Single-molecule bioelectrocatalysis - multi-copper nitrite reductase and laccases.

Documents:
alicante.pdf

Related event

Electrocatalysis of interfacial bioelectrochemical electron transfer processes at the single-molecule level: Invited keynote/tutorial communication, FP7 Marie Curie Training Network Programme ELCAT, University of Alicante
14/09/2011 → 17/09/2011
Alicante, Spain
Activity: Talks and presentations › Conference presentations

Electrocatalysis of interfacial bioelectrochemical electron transfer processes at the single-molecule level
Period: 14 Sep 2011 → 17 Sep 2011
Jens Ulstrup (Keynote speaker)
Department of Chemistry
NanoChemistry

Description
The structure, two-dimensional surface organization, and electron transfer (ET) function of biological macromolecules and biomimetic molecules on solid surfaces can now be addressed at a degree of detail that reaches the level of the single molecule. ET metalloproteins such as blue copper, heme, and iron-sulfur proteins have thus become new target molecules for single-molecule electrochemical surface science. Redox molecules such as these are "smart" molecules in the sense that they can be brought to "do" something in their natural aqueous biological buffer environment. Scanning tunnelling and atomic force microscopy in aqueous biological media supported by theoretical frames are core approaches in these new areas. We overview here some new recent efforts in electrocatalysis of redox metalloenzymes and biomimetic metalloenzyme models also brought to the single-molecule level. Structures and enzyme mechanisms of these large and composite biomolecular entities offer new challenges. We shall address: • Binding modes of molecular linkers on electrochemical Au(111)-electrode surfaces. • A biomimetic metalloenzyme unit – the [Mo3S4]3+/4+ cluster. • Interfacial bioelectrochemical catalysis by "normal" and "green" gold nanoparticles. • Single-molecule bioelectrocatalysis - multicopper nitrite reductase and laccases.
Invited lecture

Conference on analytical chemistry

Documents:
The Principle of Pooled Calibrations and Outlier Retainment Elucidates Optimum Performance of Ion Chromatography

Related event

Euroanalysis 16: Challenges in Modern Analytical Chemistry
Belgrade, Serbia
Activity: Talks and presentations › Conference presentations

Euroanalysis 16
Period: 11 Sep 2011 → 15 Sep 2011
Jens Andersen (Chairman)
Department of Chemistry
Analytical Chemistry

Description
Session on quality assurance
Chairman of session on quality assurance

Related event

Euroanalysis 16: Challenges in Modern Analytical Chemistry
Belgrade, Serbia
Activity: Attending an event › Participating in or organising a conference

Scientific committee (External organisation)
Period: 11 Sep 2011 → 15 Sep 2011
Jens Andersen (Participant)
Department of Chemistry
Analytical Chemistry

Description
Euroanalysis 16, Belgrade, Serbia
Degree of recognition: International

Related external organisation
Scientific committee
Activity: Membership › Membership of committees, commissions, boards, councils, associations, organisations, or similar

10th EuropaCat Congress
Period: 28 Aug 2011 → 2 Sep 2011
Helene Kolding (Participant)
Department of Chemistry
Centre for Catalysis and Sustainable Chemistry

Related event

10th EuropaCat Congress
28/08/2011 → 02/09/2011
Glasgow, United Kingdom
Activity: Attending an event › Participating in or organising a conference
New approaches to single-molecule science 2: Bioelectrochemistry of single molecules: Invited Graduate student and staff seminar, Molecular Science and Engineering College, Shandong, University
Period: 22 Jul 2011
Jens Ulstrup (Speaker)
Department of Chemistry
NanoChemistry

Related external organisation

Unknown external organisation
Activity: Talks and presentations › Conference presentations

New approaches to single-molecule science 1: Bioelectrochemistry of single molecules: Invited Summer school undergraduate tutorial, Molecular Science and Engineering College, Shandong, University
Jens Ulstrup (Speaker)
Department of Chemistry
NanoChemistry

Related external organisation

Unknown external organisation
Activity: Talks and presentations › Conference presentations

Femtochemistry: theory and simulation
Period: 27 May 2011
Klaus Braagaard Møller (Invited speaker)
Department of Chemistry
Physical and Biophysical Chemistry

Description
Quantum Dynamics Seminar, Max Planck Institute for the Physics of Complex Systems, Dresden, Germany

Related external organisation

Unknown external organisation
Activity: Talks and presentations › Conference presentations

Bioelectrochemistry of single molecules: Invited talk, Nanotechnology Center, Shanghai University
Period: 24 May 2011
Jens Ulstrup (Speaker)
Department of Chemistry
NanoChemistry

Description
Place: Shanghai

Related external organisation

Unknown external organisation
Activity: Talks and presentations › Conference presentations

Ph.D. Evaluation Committee (External organisation)
Period: 5 Jan 2011 → 12 Nov 2012
Jens Andersen (Participant)
Department of Chemistry
Analytical Chemistry

Description
University of Copenhagen

Evaluation of Ph.D. Thesis
Body type: University

Related external organisation
Ph.D. Evaluation Committee
Activity: Membership › Membership of committees, commissions, boards, councils, associations, organisations, or similar

Thermodynamic modeling of sour gas cleaning process with alkanolamine: Oral presentation at the 25th European SYmposium on Applied Thermodynamics (ESAT), St.Petersburg, Russia
Period: 1 Jan 2011 → …
Erling Halfdan Stenby (Speaker)
Department of Chemistry
Center for Energy Resources Engineering

Related external organisation
Unknown external organisation
Activity: Talks and presentations › Conference presentations

Thermodynamic modeling of sour gas cleaning process with alkanolamine: Presented at (oral presentation) CERE discussion meeting, Hillerød
Period: 1 Jan 2011 → …
Erling Halfdan Stenby (Speaker)
Department of Chemistry
Center for Energy Resources Engineering

Related external organisation
Unknown external organisation
Activity: Talks and presentations › Conference presentations

Single-molecule conductivity of redox metalloproteins and metalloenzymes in biological media
Period: 9 Dec 2010
Jens Ulstrup (Invited speaker)
Department of Chemistry
NanoChemistry

Related external organisation
University of New South Wales
Sydney, Australia
Activity: Talks and presentations › Guest lectures, external teaching and course activities at other universities

Single-molecule conductivity of redox molecules and metalloproteins in biological media
Period: 24 Sep 2010
Jens Ulstrup (Invited speaker)
Department of Chemistry
NanoChemistry

**Related event**

**Scandinavian Workshop on Single-molecule NanoScience**
24/09/2010 → …
Denmark
Activity: Talks and presentations › Conference presentations

**Grøn Dyst**
Period: 25 Jun 2010
Helene Kolding (Participant)
Department of Chemistry
Centre for Catalysis and Sustainable Chemistry

**Related event**

**Grøn Dyst: DTU's studiekonference om bæredygtighed, klimateknologi og miljø**
25/06/2010 → 25/06/2010
Kongens Lyngby, Denmark
Activity: Attending an event › Participating in or organising a conference

**Electronic single-molecule conductivity of redox proteins and metalloenzymes in biological media**
Period: 22 Jun 2010 → 26 Jun 2010
Jens Ulstrup (Speaker)
Department of Chemistry
NanoChemistry

**Description**
Electronic single-molecule conductivity of redox proteins and metalloenzymes in biological media: Workshop on Transport Phenomena in Molecular Nanostructures. Book of abstracts

ETH Zürich CECAM (Centre Européen de Calcul Atomique et Moleculaire)

**Related external organisation**

**ETH Zurich**
Zürich, Switzerland
Activity: Talks and presentations › Conference presentations

**Electronic single-molecule conductivity of redox proteins and metalloenzymes in biological media**
Period: 22 Jun 2010 → 26 Jun 2010
Jingdong Zhang (Speaker)
Department of Chemistry
NanoChemistry

**Description**
Electronic single-molecule conductivity of redox proteins and metalloenzymes in biological media: Workshop on Transport Phenomena in Molecular Nanostructures. Book of abstracts
22/06/2010 → 26/06/2010
ETH Zürich CECAM (Centre Européen de Calcul Atomique et Moleculaire)

**Related external organisation**

**ETH Zurich**
Zürich, Switzerland
Activity: Talks and presentations › Conference presentations
Electronic single-molecule conductivity of redox proteins and metalloenzymes in biological media
Period: 22 Jun 2010 → 26 Jun 2010
Qijin Chi (Speaker)
Department of Chemistry
NanoChemistry

Description
Electronic single-molecule conductivity of redox proteins and metalloenzymes in biological media: Workshop on Transport Phenomena in Molecular Nanostructures. Book of abstracts
22/06/2010 → 26/06/2010
ETH Zürich CECAM (Centre Européen de Calcul Atomique et Moléculaire)

Related external organisation
ETH Zurich
Zürich, Switzerland
Activity: Talks and presentations › Conference presentations

Theory and Simulation of Time-resolved X-ray Diffraction
Period: 25 Feb 2010 → 28 Feb 2010
Klaus Braagaard Møller (Invited speaker)
Department of Chemistry
Physical and Biophysical Chemistry

Related event
Banff Meeting on Structural Dynamics
25/02/2010 → 28/02/2010
Banff, Alberta, Canada
Activity: Talks and presentations › Conference presentations

Analytical Chemistry and Quality Assurance for Decision Making
Period: 6 Sep 2009 → 10 Sep 2009
Jens Andersen (Speaker)
Department of Chemistry
Analytical Chemistry

Related event
Euroanalysis XV
Innsbruck, Austria
Activity: Talks and presentations › Conference presentations

Euroanalysis XV
Period: 6 Sep 2009 → 10 Sep 2009
Jens Andersen (Participant)
Department of Chemistry
Analytical Chemistry

Description
Poster 'Strontium Treatment does not Affect the Mineralisation of Calcified Tissue in Rats and Dogs'

Related event
Euroanalysis XV
Innsbruck, Austria
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

39th Danish Crystallographer Meeting and 2nd DanScatt Annual Meeting
Period: 2 Jun 2009 → 3 Jun 2009
Jens Andersen (Participant)
Department of Chemistry
Analytical Chemistry

Description
Poster, 'Dehydration Properties of Strontium Ranelate', Kenny Ståhl, Christian G. Hartmann, Carsten B. Prag, Søren R. Sørensen, Anders C. Raffalt, Stephan Christgau and Jens E.T. Andersen

Related event
39th Danish Crystallographer Meeting and 2nd DanScatt Annual Meeting
02/06/2009 → 03/06/2009
Lyngby, Denmark
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

39th Danish Crystallographer Meeting and 2nd DanScatt Annual Meeting
Period: 2 Jun 2009 → 3 Jun 2009
Jens Andersen (Participant)
Department of Chemistry
Analytical Chemistry

Description
Poster, 'Locating Strontium Ions in Bone Tissue using EXAFS', C.G. Hartmann, J.E.T. Andersen and K. Ståhl

Related event
39th Danish Crystallographer Meeting and 2nd DanScatt Annual Meeting
02/06/2009 → 03/06/2009
Lyngby, Denmark
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Theory and application of time-resolved x-ray diffraction
Period: 2 Jun 2009 → 3 Jun 2009
Klaus Braagaard Møller (Invited speaker)
Department of Chemistry
Physical and Biophysical Chemistry

Related event
39th Danish Crystallographer Meeting
02/06/2009 → 03/06/2009
Lyngby, Denmark
Activity: Talks and presentations › Conference presentations

EuCheMS-DAC Symposium on Analytical Chemistry
Period: 20 Apr 2009
Jens Andersen (Participant)
Department of Chemistry
Analytical Chemistry

Description
Talk, 'Making Decisions by Analytical Chemistry'
EuCheMS-DAC Symposium on Analytical Chemistry
EuCheMS-DAC Symposium on Analytical Chemistry
19/04/2009 → 20/04/2009
Tallinn, Estonia
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

214th Meeting of The Electrochemical Society
Jens Andersen (Invited speaker)
Department of Chemistry
Analytical Chemistry

Description
Invited speaker, 'Correspondence between Experiment and Theory of Bulk Electrocrystallisation at Solid Electrodes in Aqueous Electrolyte'

214th Meeting of The Electrochemical Society
Period: 12/10/2008 → 17/10/2008
Honolulu, HI, United States
Activity: Talks and presentations › Conference presentations

8th Nordic Femtochemistry Meeting
Klaus Braagaard Møller (Organizer)
Department of Chemistry
Physical and Biophysical Chemistry

8th Nordic Femtochemistry Meeting
Period: 02/10/2008 → 04/10/2008
Knebel, Denmark
Activity: Attending an event › Participating in or organising a conference

National Danish Symposium on Analytical Chemistry
Jens Andersen (Chairman)
Department of Chemistry
Analytical Chemistry

Description
National Danish Symposium on Analytical Chemistry
Degree of recognition: National

National Danish Symposium on Analytical Chemistry
Period: 18/08/2008 → 20/08/2008
Kgs. Lyngby, Denmark
Activity: Attending an event › Participating in or organising a conference

Nuklear måleusikkerhed (IDA): Fra Risø Rapport No. 1 til Akkreditering nrr. 488
Period: 27 Mar 2008
Kaj Heydorn (Speaker)
Department of Chemistry

Documents:
IDA-foredrag 2008.pdf

Related external organisation

The Danish Society of Engineers, IDA
Kalvebod Brygge 31-33, DK-1780, Copenhagen V, Denmark
Activity: Talks and presentations › Guest lectures, external teaching and course activities at other universities

European Association of Chemical and Molecular Sciences Division of Analytical Chemistry (External organisation)
Period: 1 Oct 2007 → 31 Dec 2012
Jens Andersen (Secretary)
Department of Chemistry
Analytical Chemistry

Description
Associaation of European Analytical Chemists in Academia
Degree of recognition: International

Related external organisation

European Association of Chemical and Molecular Sciences Division of Analytical Chemistry
Activity: Membership › Membership of committees, commissions, boards, councils, associations, organisations, or similar

Euroanalysis XIV
Period: 10 Sep 2007 → 14 Sep 2007
Jens Andersen (Participant)
Department of Chemistry
Analytical Chemistry

Description
Poster, 'Determination of Strontium by ICP-MS and a Study of the Influence on Native Elements in Incisors of Rats' Søren R. Sørensen, Anders C. Raffalt, Jens E.T. Andersen and Stephan Christgau

Related event

Euroanalysis XIV
Antwerp, Belgium
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Euroanalysis XIV
Period: 10 Sep 2007 → 14 Sep 2007
Jens Andersen (Invited speaker)
Department of Chemistry
Analytical Chemistry

Description
Invited speaker, 'A Course at the Master Level Demonstrating Quality Assurance by Spectrophotometric Determination of Iron in two Experiments'
Related event

Euroanalysis XIV
Antwerp, Belgium
Activity: Talks and presentations › Conference presentations

2nd AcadeMiC Summer School on Education in Metrology in Chemistry
Jens Andersen (Participant)
Department of Chemistry
Analytical Chemistry

Description
Poster, ‘Statistical Control in Analytical Chemistry by Prediction of Uncertainties’

Related event

2nd AcadeMiC Summer School on Education in Metrology in Chemistry
23/06/2007 → 26/06/2007
Wieliczka, Poland
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

2nd AcadeMiC Summer School on Education in Metrology in Chemistry
Jens Andersen (Invited speaker)
Department of Chemistry
Analytical Chemistry

Description
Invited speaker, ‘Analytical Chemistry in the European Higher Education Area’

Related event

Chemical dynamics: Theory and simulation
Period: 2006
Klaus Braagaard Møller (Invited speaker)
Department of Chemistry
Physical and Biophysical Chemistry

Related event

KAIST Lecture Series
01/01/2006 → …
Korea Advanced Institute of Science and Technology, Denmark
Activity: Talks and presentations › Conference presentations

Dissipative dynamics: Hydrodynamic and mixed representations
Period: 2006
Klaus Braagaard Møller (Invited speaker)
Department of Chemistry
Physical and Biophysical Chemistry
Related event

**Workshop on Dynamics of Open Quantum Systems**
Bangor, Denmark
Activity: Talks and presentations › Conference presentations

**Femtochemistry: Theory and simulation**
Period: 2006
Klaus Braagaard Møller (Invited speaker)
Department of Chemistry
Physical and Biophysical Chemistry

Related event

**AMO Physics Seminar**
01/01/2006 → …
University of Aarhus, Denmark
Activity: Talks and presentations › Conference presentations

**1st European Chemistry Congress**
Jens Andersen (Participant)
Department of Chemistry
Analytical Chemistry

Description
Poster, 'Incorporation of Strontium in Bone and Teeth of Dogs after one Month Treatment with Strontium Malonate', Anders C. Raffalt, Stephan Christgau and Jens E.T. Andersen

Related event

**1st European Chemistry Congress**
Budapest, Hungary
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

**23rd European Crystallography Meeting**
Period: 1 Aug 2006 → 2 Aug 2006
Jens Andersen (Participant)
Department of Chemistry
Analytical Chemistry

Description
Abstract, 'Isostructural strontium formate, fumarate and acetyldicarboxylate' Kenny Ståhl, Jens E.T. Andersen and Stephan Christgau

Related event

**23rd European Crystallography Meeting**
Leuven, Belgium
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

**IOF World Congress on Osteoporosis 2006**
Period: 2 Jun 2006 → 6 Jun 2006
Jens Andersen (Participant)
Department of Chemistry
Analytical Chemistry

Description
Poster, 'Partial Restoration of Skeletal Strength in Ovariectomized Rats by Treatment With Strontium Salts’, Stephan Christgau, Pernille Høegh Andersen and Jens E.T. Andersen

IOF World Congress on Osteoporosis

Related event
IOF World Congress on Osteoporosis 2006
02/06/2006 → 06/06/2006
Toronto, Canada
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Dynamics of coupled Bohmian and phase-space variables
Period: 2005
Klaus Braagaard Møller (Invited speaker)
Department of Chemistry
Physical and Biophysical Chemistry

Related event
Workshop on Quantum Dynamics of Complex Molecular Systems
18/05/2005 → 20/05/2005
Paris, France
Activity: Talks and presentations › Conference presentations

EuCheMS Division of Analytical Chemistry (External organisation)
Period: 2005 → 2012
Jens Andersen (Participant)
Department of Chemistry
Analytical Chemistry

Description
Member of Steering Committee

Body type: Academic Society
Degree of recognition: International

Related external organisation
EuCheMS Division of Analytical Chemistry
Activity: Membership › Membership of committees, commissions, boards, councils, associations, organisations, or similar

Quantum hydrodynamic moment expansions: A bridge between phase space distributions and Bohmian mechanics
Period: 2004
Klaus Braagaard Møller (Invited speaker)
Department of Chemistry
Physical and Biophysical Chemistry

Related event
Quantum Molecular Dynamics for Condensed Phase Applications : CECAM Workshop
16/09/2004 → 18/09/2004
Lyon, France
Activity: Talks and presentations › Conference presentations
206th Meeting of the Electrochemical Society
Period: 3 Oct 2004 → 8 Oct 2004
Jens Andersen (Invited speaker)
Department of Chemistry
Analytical Chemistry

Description
Invited speaker, 'Imaging by Electrochemical Scanning Tunneling Microscopy and Deconvolution Resolving More Details of Surfaces Nanomorphology'

Related event
206th Meeting of the Electrochemical Society : 5th International Symposium on Ionic and 5th International Symposium on Ionic and mixed Conducting Ceramics
03/10/2004 → 08/10/2004
Honolulu, HI, United States
Activity: Talks and presentations › Conference presentations

8th European Conference on Analytical Chemistry
Period: 5 Sep 2004
Jens Andersen (Participant)
Department of Chemistry
Analytical Chemistry

Description
Oral presentation, 'Filterless Preconcentration, Flow Injection Analysis and Detection by Inductively-Coupled-Plasma Mass Spectrometry'

Related event
8th European Conference on Analytical Chemistry: The Role of Analytical Chemistry in the protection of the Citizens
05/09/2004 → 10/09/2004
Salamanca, Spain
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

8th European Conference on Analytical Chemistry
Period: 5 Sep 2004 → 10 Sep 2004
Jens Andersen (Invited speaker)
Department of Chemistry
Analytical Chemistry

Description
Invited speaker, 'Physics in the Model for a Eurobachelor Syllabus, Euroanalysis XIII'

Related event
8th European Conference on Analytical Chemistry: The Role of Analytical Chemistry in the protection of the Citizens
05/09/2004 → 10/09/2004
Salamanca, Spain
Activity: Talks and presentations › Conference presentations

Ultrafast IR spectroscopy of water: A theoretical study
Period: 2003
Klaus Braagaard Møller (Invited speaker)
Department of Chemistry
Physical and Biophysical Chemistry

Related event

Kemisk Forenings Årsmøde
12/06/2003 → …
Odense, Denmark
Activity: Talks and presentations › Conference presentations

Trajectories in phase space: Hydrodynamics vs. Liouville space
Period: 2002
Klaus Braagaard Møller (Invited speaker)
Department of Chemistry
Physical and Biophysical Chemistry

Related event

Currents, Trajectories and Applications in Quantum Dynamics: CECAM Workshop
01/01/2002 → …
Denmark
Activity: Talks and presentations › Conference presentations

21st European Congress on Surface Science
Jens Andersen (Participant)
Department of Chemistry
Analytical Chemistry

Description

Related event

21st European Congress on Surface Science
24/06/2002 → 28/06/2002
Malmö, Sweden
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

21st European Congress on Surface Science
Jens Andersen (Participant)
Department of Chemistry
Analytical Chemistry

Description

Related event

21st European Congress on Surface Science
24/06/2002 → 28/06/2002
Malmö, Sweden
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

21. Arbejdsseminar i Atomspektrometri
Jens Andersen (Invited speaker)
Department of Chemistry
Analytical Chemistry

Description
Metoder til Opkoncentrering af Metalioner med FIA og Analyse med AAS

Related event
21. Arbejdsseminar i Atomspektrometri
21/10/2001 → 23/10/2001
Røros, Norway
Activity: Talks and presentations › Conference presentations

Ulstrup Symposium on Bioinorganic Chemistry, Condensed Matter Chemical Physics at Atomic Resolution
Period: 12 Oct 2001
Jens Andersen (Organizer)
Department of Chemistry
Analytical Chemistry

Description
Chairman
Ulstrup Symposium on Bioinorganic Chemistry, Condensed Matter Chemical Physics at Atomic Resolution

Related event
Ulstrup Symposium on Bioinorganic Chemistry, Condensed Matter Chemical Physics at Atomic Resolution
12/10/2001 → …
Copenhagen, Denmark
Activity: Attending an event › Participating in or organising a conference

10th International Conference on Bioinorganic Chemistry
Period: 10 Aug 2001
Jens Andersen (Participant)
Department of Chemistry
Analytical Chemistry

Description

Related event
10th International Conference on Bioinorganic Chemistry
26/08/2001 → 31/08/2001
Florence, Italy
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Meeting at DTU Microelectronics Center
Period: 20 Feb 2001
Jens Andersen (Speaker)
Department of Chemistry
Analytical Chemistry

Description
Talk 'In situ Scanning Tunnelling Microscopy'

Meeting at DTU Microelectronics Center
Related event

Meeting at DTU Microelectronics Center
20/02/2001 → …
Kgs. Lyngby, Denmark
Activity: Talks and presentations › Conference presentations

Danish Society of Analytical Chemistry (External organisation)
Period: 2000 → 2012
Jens Andersen (Member)
Department of Chemistry
Analytical Chemistry

Description
Delegate to EuCheMS Division of Analytical Chemistry

Body type: Academic Society
Degree of recognition: International

Related external organisation

Danish Society of Analytical Chemistry
Activity: Membership › Membership of committees, commissions, boards, councils, associations, organisations, or similar

7th International Frumkin Symposium
Jens Andersen (Participant)
Department of Chemistry
Analytical Chemistry

Description

Related event

7th International Frumkin Symposium: Basic Electrochemistry for Science and Technology
23/10/2000 → 28/10/2000
Moscow, Russian Federation
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

51st International Society of Electrochemistry Meeting
Period: 3 Sep 2000 → 8 Sep 2000
Jens Andersen (Participant)
Department of Chemistry
Analytical Chemistry

Description

Related event

51st International Society of Electrochemistry Meeting
03/09/2000 → 08/09/2000
Warzaw, Poland
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.
6th National Danish Congress on Analytical Chemistry
Jens Andersen (Participant)
Department of Chemistry
Analytical Chemistry

Related event
6th National Danish Congress on Analytical Chemistry
16/08/2000 → 17/08/2000
Copenhagen, Denmark
Activity: Attending an event › Participating in or organising a conference

5th Europ Biological Inorganic Chemistry Conference
Jens Andersen (Participant)
Department of Chemistry
Analytical Chemistry

Description

Related event
5th Europ Biological Inorganic Chemistry Conference
17/07/2000 → 20/07/2000
Toulouse, France
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Faraday Discussion 116
Jens Andersen (Participant)
Department of Chemistry
Analytical Chemistry

Description

Faraday Discussion 116: Bioelectrochemistry, Royal Society of Chemistry

Related event
Faraday Discussion 116: Bioelectrochemistry
17/07/2000 → 19/07/2000
Southampton, United Kingdom
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

8th Fischer Symposium
Jens Andersen (Participant)
Department of Chemistry
Analytical Chemistry

Description
J. Zhang, Q. Chi, J.E.T. Andersen, A.G. Hansen, J.U. Nielsen and J. Ulstrup, 'Adsorption of Amino Acids and Redox Metalloproteins at Single-Crystal Electrodes Investigated by Electrochemical Methods and In Situ STM'

Related event

8th Fischer Symposium
18/06/2000 → 22/06/2000
Karlsruhe, Germany
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Volkswagen-Schwerpunkt – Intra- und intermolekulare
Jens Andersen (Participant)
Department of Chemistry
Analytical Chemistry

Description

Related event

Volkswagen-Schwerpunkt – Intra- und intermolekulare
04/06/2000 → 06/06/2000
Wildbad Kreuth, Germany
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

In Situ Nanoscale Biochemistry by SPM-based Technologies
Jens Andersen (Participant)
Department of Chemistry
Analytical Chemistry

Description
Poster, Kinetics of the Self-assembly of Alkanethiols on a Gold Coated Microcantilever, A.G. Hansen, J.E.T. Andersen, J. Ulstrup and A. Boisen

Related event

In Situ Nanoscale Biochemistry by SPM-based Technologies
15/03/2000 → 18/03/2000
Kgs. Lyngby, Denmark
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

In Situ Nanoscale Biochemistry by SPM-based Technologies
Jens Andersen (Participant)
Department of Chemistry
Analytical Chemistry

Description

Related event

In Situ Nanoscale Biochemistry by SPM-based Technologies
15/03/2000 → 18/03/2000
Kgs. Lyngby, Denmark
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

**In Situ Nanoscale Biochemistry by SPM-based Technologies**
Jens Andersen (Participant)
Department of Chemistry
Analytical Chemistry

**Description**
Talk, presented by Q. Chi, 25 min., Creating Nanoscale Pits and Patterns on Solid Surfaces in Liquid Environment by STM, Q. Chi, J. Zhang, E.P. Friis, J.E.T. Andersen and J. Ulstrup

**Related event**

**In Situ Nanoscale Biochemistry by SPM-based Technologies**
15/03/2000 → 18/03/2000
Kgs. Lyngby, Denmark
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

**In Situ Nanoscale Biochemistry by SPM-based Technologies**
Jens Andersen (Organizer)
Department of Chemistry
Analytical Chemistry

**Description**
Workshop on In Situ Nanoscale Biochemistry by SPM-Based Technologies, ISNB-2000

**Related event**

**Probe Microscopy (Journal)**
Jens Andersen (Reviewer)
Department of Chemistry
Analytical Chemistry

**Description**
Workshop on In Situ Nanoscale Biochemistry by SPM-Based Technologies, ISNB-2000

11 Refereed contributions from the International Workshop 2000

**Related journal**

**Probe Microscopy**
1355-185X
BFI (2008): BFI-level 1, Scopus rating (2004): SJR 0.533 SNIP 0.515
Central database
Activity: Research › Journal editor

**Annual meeting of the Danish Society of Electrochemistry**
Period: 9 Dec 1999
Jens Andersen (Participant)
Department of Chemistry
Analytical Chemistry

**Description**
Talk, 90 min., A look into the world of Nano-electrochemistry by in situ Scanning Probe Microscopy (in situ SPM)

**Related event**

*Annual meeting of the Danish Society of Electrochemistry*
09/12/1999 → …
Kgs. Lyngby, Denmark
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

7th International Seminar on Electroanalytical Chemistry
Jens Andersen (Participant)

Department of Chemistry
Analytical Chemistry

**Description**

**Related event**

7th International Seminar on Electroanalytical Chemistry
22/10/1999 → 24/10/1999
Changchun, China
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

7th International Seminar on Electroanalytical Chemistry
Jens Andersen (Participant)

Department of Chemistry
Analytical Chemistry

**Description**

**Related event**

7th International Seminar on Electroanalytical Chemistry
22/10/1999 → 24/10/1999
Changchun, China
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

**Electrochemistry and Superstructures**
Period: 11 Jun 1999
Jens Andersen (Lecturer)

Department of Chemistry
Analytical Chemistry

**Related event**

**Meeting at DTU IPU**
11/06/1999 → …
Kgs. Lyngby, Denmark
Activity: Talks and presentations › Conference presentations

**Electrochemistry on metalloproteins and related subjects – a joint MIC/IK seminar**
Period: 3 Feb 1999
Jens Andersen (Lecturer)
Department of Chemistry
Analytical Chemistry

**Related event**

**Electrochemistry on metalloproteins and related subjects – a joint MIC/IK seminar**
03/02/1999 → …
Kgs. Lyngby, Denmark
Activity: Talks and presentations › Conference presentations

**Danish Society of Analytical Chemistry (External organisation)**
Period: 1998 → 1999
Jens Andersen (Chairman)
Department of Chemistry
Analytical Chemistry

**Description**
Body type: Academic Society

**Related external organisation**

**Danish Society of Analytical Chemistry**
Activity: Membership › Membership of committees, commissions, boards, councils, associations, organisations, or similar

**14th National Conference on Analytical Chemistry**
Jens Andersen (Participant)
Department of Chemistry
Analytical Chemistry

**Description**
Poster, presented by Elena Diacu, XIVth National Conference on analytical chemistry, SCAR ’98, J.E.T. Andersen and Elena Diacu

**Related event**

**14th National Conference on Analytical Chemistry**
Piatra Neamt, Romania
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

**Euroanalysis X**
Jens Andersen (Speaker)
Department of Chemistry
Analytical Chemistry

**Description**

**Related event**
Euroanalysis X
Basel, Switzerland
Activity: Talks and presentations › Conference presentations

Danish Society of Analytical Chemistry (External organisation)
Jens Andersen (Participant)
Department of Chemistry
Analytical Chemistry

Description
Treasurer

Body type: Academic Society

Related external organisation
Danish Society of Analytical Chemistry
Activity: Membership › Membership of committees, commissions, boards, councils, associations, organisations, or similar

ESF Workshop on Bioelectrochemistry
Period: 9 May 1996 → 11 May 1996
Jens Andersen (Organizer)
Department of Chemistry
Analytical Chemistry

Related event
ESF Workshop on Bioelectrochemistry
09/05/1996 → 11/05/1996
Copenhagen, Denmark
Activity: Attending an event › Participating in or organising a conference

The Snowdonian Conference of Electrified Interfaces
Jens Andersen (Other)
Department of Chemistry
Analytical Chemistry

Description
Poster, Jens E.T. Andersen, Marianne H. Jensen, Lars L. Madsen, Per Møller and Jens Ulstrup 'Perspectives for in-situ Scanning Tunnelling Microscopy of Metalloproteins'

Related event
The Snowdonian Conference of Electrified Interfaces
16/07/1995 → 21/07/1995
United Kingdom
Activity: Talks and presentations › Conference presentations

The Snowdonian Conference of Electrified Interfaces
Jens Andersen (Participant)
Department of Chemistry
Analytical Chemistry
Related event

The Snowdonian Conference of Electrified Interfaces
16/07/1995 → 21/07/1995
United Kingdom
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Danish Electrochemistry Society's 25-Year Jubilee Symposium
Period: 9 Jun 1995
Jens Andersen (Participant)
Department of Chemistry
Analytical Chemistry
Description
Poster 'In situ STM'

Related event

Danish Electrochemistry Society's 25-Year Jubilee Symposium
09/06/1995 → …
Kgs. Lyngby, Denmark
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

ESF Workshop on Bioelectrochemistry
Jens Andersen (Invited speaker)
Department of Chemistry
Analytical Chemistry
Description
Talk, 30 min., ' Immobilised Cytochrome c imaged by in situ STM '

Related event

ESF Workshop on Bioelectrochemistry
09/05/1995 → 11/05/1995
Copenhagen, Denmark
Activity: Talks and presentations › Conference presentations

European Congress on in situ STM/AFM
Period: 1994
Jens Andersen (Organizer)
Department of Chemistry
Analytical Chemistry
Description
European Congress on in situ STM/AFM

Related event

European Congress on in situ STM/AFM
15/02/1994 → 16/02/1994
Copenhagen, Denmark
Activity: Attending an event › Participating in or organising a conference

European Congress on in situ STM/AFM
Period: 15 Feb 1994 → 16 Feb 1994
Jens Andersen (Organizer)
Description
European Congress on in situ STM/AFM

Related event
European Congress on in situ STM/AFM
15/02/1994 → 16/02/1994
Copenhagen, Denmark
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

DME A/S Meeting for Application Engineers
Period: 1 Jan 1994 → 1 Dec 1994
Jens Andersen (Speaker)
Department of Chemistry
Analytical Chemistry

Related event
DME A/S Meeting for Application Engineers
01/08/1994 → …
Herlev, Denmark
Activity: Talks and presentations › Conference presentations

1st European Congress on Catalysis
Period: 1 Sep 1993 → 30 Sep 1993
Jens Andersen (Participant)
Department of Chemistry
Analytical Chemistry

Description
Author

Related event
1st European Congress on Catalysis
12/09/1993 → 17/09/1993
Montpellier, France
Activity: Attending an event › Participating in or organising workshops, courses, seminars etc.

Prizes:

Honours student: Advanced and Applied Chemistry: Catalysis and Nanotechnology
Helene Kolding (Recipient)
Centre for Catalysis and Sustainable Chemistry, Department of Chemistry

Description
1 Sept 2009 - 17 Nov 2011

Details
Awarded date: 17 Nov 2011
Granting Organisations: Technical University of Denmark
Prize: Prizes, scholarships, distinctions
Otto-Mønsted travel grant
Arnab Halder (Recipient)
Department of Chemistry, NanoChemistry, Organic Chemistry

Description
Travel grant for attending international conference.

Details
Awarded date: Aug 2016
Prize: Prizes, scholarships, distinctions

Poul V. Andersen Foundation grant
Arnab Halder (Recipient) & Suhith Hemanth (Recipient)
Department of Chemistry, NanoChemistry, Organic Chemistry, Department of Micro- and Nanotechnology

Description
The project “3D Nanocarbon chips for microsupercapacitors and ultrasensitive detection” by PhD students Arnab Halder from DTU Chemistry and Suhith Hemanth from DTU Nanotech has been selected as the winning project by the Poul V. Andersen Foundation and will receive a grant of 250,000 DKK. Only one project per year is awarded by the Poul V. Andersen Foundation.

Details
Awarded date: 29 Feb 2016
Granting Organisations: Technical University of Denmark
Prize: Prizes, scholarships, distinctions

‘The Best Oral Presentation’ at DTU Chemistry PhD symposium 2016
Arnab Halder (Recipient)
Department of Chemistry, NanoChemistry, Organic Chemistry

Details
Awarded date: 10 Nov 2016
event: DTU Chemistry PhD Symposium 2016
Prize: Prizes, scholarships, distinctions

Press clippings:

Solving a nanotechnology riddle – what makes gold atoms stick together
Arnab Halder & Jens Ulstrup
02/03/2016

Description
NanoChemistry, Department of Chemistry

Media coverage (1)

Solving a nanotechnology riddle – what makes gold atoms stick together
02/03/2016
Highlights of our PNAS paper
http://www.pnas.org/content/113/11/E1424
Arnab Halder & Jens Ulstrup
NanoChemistry, Department of Chemistry

Relations
Research outputs:
Gold surfaces and nanoparticles are protected by Au(0)-thiol species and are destroyed when Au(I)-thiolates form
Press / Media
Gold nanoparticles riddle solved – offering medical hope
Arnab Halder & Jens Ulstrup
01/03/2016

Description
https://www.scimex.org/newsfeed/gold-nanoparticles-riddle-solved-offering-medical-hope
NanoChemistry, Department of Chemistry

Media coverage (1)
Gold nanoparticles riddle solved – offering medical hope
01/03/2016
Australia
https://www.scimex.org/newsfeed/gold-nanoparticles-riddle-solved-offering-medical-hope
https://www.scimex.org/newsfeed/gold-nanoparticles-riddle-solved-offering-medical-hope
Arnab Halder & Jens Ulstrup
NanoChemistry, Department of Chemistry

Relations
Research outputs:
Gold surfaces and nanoparticles are protected by Au(0)-thyl species and are destroyed when Au(I)-thiolates form

First-of-its kind solution to the challenge of storing hydrogen fuel
Martin Nielsen
09/09/2013
Organic Chemistry, Department of Chemistry, Centre for Catalysis and Sustainable Chemistry

Media contribution (1)
First-of-its kind solution to the challenge of storing hydrogen fuel
09/09/2013
ACSLive, Television
http://www.ustream.tv/recorded/38499323
Martin Nielsen
Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry

Dansk forsker: Biomasse kan blive en guldgrube
Martin Nielsen
23/03/2013

Subject
Renewables
Organic Chemistry, Department of Chemistry, Centre for Catalysis and Sustainable Chemistry

Media contribution (1)
Dansk forsker: Biomasse kan blive en guldgrube
23/03/2013
Ingeniøren, Print
Regner Hansen
http://ing.dk/artikel/dansk-forsker-biomasse-kan-blive-en-guldgrube-157302
Martin Nielsen
Department of Chemistry, Centre for Catalysis and Sustainable Chemistry, Organic Chemistry

Smill Du er på. http://emagstudio.win.dtu.dk/E-books/DTU-Avisen/DTUavis0112/#/20/
Anastasia Aleksandrovna Permyakova
01/01/2012

Description
http://emagstudio.win.dtu.dk/E-books/DTU-Avisen/DTUavis0112/#/20/
Energy and Materials, Department of Energy Conversion and Storage, Proton conductors
Media contribution (1)
01/01/2012
DTU Avisen, Print
Charlotte Malasse
http://emagstudio.win.dtu.dk/E-books/DTU-Avisen/DTUavis0112/#/20/
Anastasia Aleksandrovna Permyakova
Department of Energy Conversion and Storage, Proton conductors, Energy and Materials
Press / Media

Jyllandsposten: Blodtud til rygeradvokat
Jens Andersen
13/10/2011
Analytical Chemistry, Department of Chemistry

Media contribution (1)
Jyllandsposten: Blodtud til rygeradvokat
13/10/2011
København, Print
Jens Andersen
Department of Chemistry, Analytical Chemistry
Press / Media

Hellere nr. 1 på Isotoplaboratoriet end nr. 2 i Direktionen (Museumsrapport); 2007: Et erindringsinterview
Kaj Heydorn
15/01/2007
Department of Chemistry

Media contribution (1)
Hellere nr. 1 på Isotoplaboratoriet end nr. 2 i Direktionen (Museumsrapport); 2007: Et erindringsinterview
15/01/2007
Bygning 207 Rum 210, Print
http://www.si.au.dk/forskning/aktuelforskning/maskinerneihaven
Kaj Heydorn
Department of Chemistry
Press / Media