Annual Report

2012

Catalysis Group – SINTEF – NTNU

KinCat
Strong Point Centre Kinetics and Catalysis

The centre was established July 1, 1998 by NTNU and SINTEF in recognition of the strong scientific level of members participating. The centre consists of the catalysis group, Department of Chemical Engineering, NTNU and the catalysis research team, SINTEF Materials and Chemistry. As of January 2008 the centre has been established as a Gemini centre by NTNU and SINTEF.

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Annual Report 2012
KINCAT
Strong Point Centre Kinetics and Catalysis

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First row: Camilla Otterlei, Andreas H. Lillebø, Ida Hjort, Farbod Dadgar, Jun Zhu, Charitha Udani, Nicla Vicinanza, Michael Wysick, Nikolaos Tsakoumis
Not present (left column):, Hilde Venvik, Trung Dung Tran, Jia Yang, Bjørn Christian Enger, Daham Sanjaya Gunawardana, De Chen.

Research Areas

- **Conversion of Natural Gas**
  - Synthesis gas and hydrogen production
  - Fischer-Tropsch synthesis
  - Dehydrogenation of ethane and propane
  - Solid acceptors for CO_2-capture
  - Production of methanol and dimethyl ether (DME)

- **Upgrading of Oil Fractions**
  - Hydrotreating
  - Catalytic reforming/isomerization

- **High Temperature Chemistry**
  - Free radical chain reactions
  - Partial oxidation of methane and NGL compounds

- **Environmental Catalysis**
  - Sulfur reduction by hydrotreating
  - Preferential oxidation of CO
  - Wastewater treatment

- **Fundamental Studies of Heterogeneous Catalysis**
  - Surface science
  - Preparation of catalytic materials (supported metals and metal oxides, zeolites, supports, nanoparticles)
  - Kinetics (steady-state and transient kinetics, SSITKA)
  - Adsorption and diffusion in porous media
  - Catalyst deactivation (sintering, coke formation)
  - Characterization of heterogeneous catalysts
  - Reactor, kinetic and first principles (DFT) modeling

- **Microstructured Reactors and Membrane Reactors**

- **Production and Application of Carbon Nanofibers**

- **Photocatalysis**
  - Water splitting.
  - Photoreforming

- **Biofuels**
  - Biomass gasification, reforming and water-gas shift
  - Bioethanol steam reforming
  - Hydrogenation of bio-oils to biofuel diesel
  - Catalytic conversion of platform molecules

Main Laboratory Equipment

❖ Reaction Laboratories

- Small pilot plants for catalytic reforming/isomerization and hydrotreating/hydrocracking
- Several set-ups for high pressure reactions as well as for reactions at atmospheric pressure
- Conventional microbalance reactors
- Oscillating microbalance reactors (TEOM)
- Dedicated laboratory for studying microreactor technology
- Membrane reactor laboratory
- CSTR reactors
- Transient kinetics (Steady-State Isotopic Transient Kinetic Analysis)
- Multireactor system for CNF synthesis

❖ Catalyst Preparation Laboratory

- Spray drier

❖ Catalyst Characterization

- Surface area (BET), porosity and pore size distributions
- Chemisorption and adsorption calorimetry
- Temperature programmed methods such as TPR, TPO and TPD
- TGA and DSC
- Raman and UV-VIS
- Acidity determination by TPD
- Scanning tunneling microscopy (STM) – in co-operation with Dept. of Physics.
- The following methods are available at NTNU:
  EM (electron microscopy), XPS (X-ray photoelectron spectroscopy), AES (auger electron spectroscopy), NMR, AFM (atomic force microscopy) and XRD (X-ray diffraction).
- Synchrotron radiation EXAFS and XRD are frequently used through ESRF and other facilities.
- Electrochemical characterization techniques

Highlights from the Activities in 2012

- Professor Jens Nørskov, Stanford University, USA was appointed Honorary Doctor at NTNU, June 1 2012. In connection with the appointment a seminar was arranged and the program is enclosed.

- Three candidates completed their PhD degrees in 2012: Hassan Jamil Dar, Eleni Patanou and Paul Radstake. The titles of the dissertations and pictures of the candidates/committees/supervisors are enclosed.

- The research laboratories that were completely renovated during 2010-11 (two floors in Chemistry hall D) have been in full operation during 2012.

- One of the group's projects underwent an external audit from Statoil on Health, Environment and Safety (HES) as well as Quality Assurance (QA). The results were very positive.

- The Group received strategic support from NTNU and participates in inGAP (Innovative Natural Gas Processes and Products). inGAP is a Centre for Research–based Innovation (SFI) appointed by the Research Council of Norway with participation from University of Oslo, SINTEF, NTNU, Statoil, Inéos, and Haldor Topsøe AS for the period 2007-2015.

- Several seminars were arranged with international participants. The programs are enclosed.

- The Group is coordinating one EU-FP7 project (FREECATS) and participates in two more European projects (CARENA, ENMIX). Members of the Group also participate in EU networks (Eurokin; BRISK - Biofuels Research Infrastructure for Sharing Knowledge). The group runs several projects within large national research programs such as GASSMAKS, NANOMAT, RENERGI, and KOSK II.

Ph.D. Candidates and Postdoctoral Projects

Nitrogen-doped carbon nanostructures as metal-free catalysts

Ph.D. Candidate: Marthe Emelie Melandsø Buan
Supervisor: Prof. Magnus Rønning
Co-supervisor: Prof. De Chen

Traditionally precious metal-based materials are used as catalysts in emerging technologies such as fuel cells, the production of light olefins and wastewater and water purification. The demand for platinum group metals and rare earth metals is hence increasing despite the already high cost and limited reserves of the catalyst materials in nature. Furthermore the high cost of the catalyst materials hinders the development and use of e.g. fuel cells in large-scale commercial applications. An essential way of reducing both the demand for noble metals and the cost of fuel cells will be the development of new metal-free catalysts capable of replacing the noble metal-based catalysts currently used. The goal of this PhD project is therefore to develop metal-free catalysts based on nitrogen-doped carbon nanostructures and apply the doped nanocarbons as electrocatalysts for the oxygen reduction reaction (ORR) in fuel cells.

The main focus of the project is nitrogen-doping of carbon nanotubes, carbon nanofibers or graphene by applying a chemical vapor deposition (CVD) method on supported growth catalysts. Optimization of the synthesis procedure to obtain catalysts with controllable nitrogen content and high surface reactivity through homogeneous dispersion of nitrogen on the material surface is essential. Chemical and physical properties of the catalyst are investigated by characterization techniques such as BET, TGA, TPR, XRD, SEM, TEM and XPS. In-situ characterization by UV-Vis, Raman and FTIR spectroscopy will be used to correlate the atomic structure of the catalyst with the catalytic activity and selectivity under industrial relevant reaction conditions. The catalytic properties of N-doped carbon nanostructures with various nitrogen concentrations and functionalization are investigated by testing the catalysts in the ORR. This is done by using electrochemical characterization techniques including cyclic voltammetry and half-cell reactions. Testing of the catalysts in the ORR is of great interest since a major objective of the project is to identify a direct relationship between the active site concentration and the catalyst performance.

Financial support:
The project is funded by NTNU and by the European Union's 7th Framework Programme through the FREECATS project.

Conversion of Synthesis Gas to Dimethyl Ether in Micro-Structured Reactors

PhD-Candidate: Farbod Dadgar
Supervisors: Prof. Hilde J. Venvik, Prof. Anders Holmen

In recent years, dimethyl ether (DME) has attracted attention as an energy carrier. DME is a promising substitute for diesel fuel, thanks to its high cetane number and low particulate matter emissions. Conventionally, DME is synthesized through a two-step process; methanol synthesis from synthesis gas ($CO+H_2$) over a copper-based catalyst and subsequent dehydration of methanol to DME over an acidic catalyst. DME can alternatively be synthesized through a one-step process by conducting both methanol synthesis and dehydration in one unit using a bi-functional catalyst, thereby alleviating the thermodynamic limitation on the methanol synthesis reaction.

Micro process technology has a potential for process intensification through equipment size reduction, process simplification and/or process integration. This along with the modularity of micro-units makes this approach interesting for on-site conversion of remote natural or biomass- derived gas. An ultimate goal could be the development of a compact gas-to-liquids technology suitable for offshore and small scale onshore applications with efficiency and cost approaching that of current large-scale productions which benefit from economy of scale. The aim of this project is to study reaction kinetics and the dual catalyst system in the direct (one-step) DME synthesis from synthesis gas. An integrated micro-structured reactor-heat exchanger is being used, which high surface-to volume ratio and micro-range flow dimensions eliminate possible heat and mass transfer limitations affecting the process.

The project is funded by the Research Council of Norway under the GASSMAKS research program (grant no. 208351/E30) and Statoil ASA through the Gas Technology Centre (NTNU/SINTEF).

Gas Phase Oxidative Dehydrogenation of Ethane: Kinetics and Reactor Simulation.

Ph.D. Candidate: Hassan J. Dar
Supervisor: Professor De Chen
Co-supervisor: Professor Hugo A. Jakobsen

Ethylene is an important intermediate in many industrial processes of petrochemicals such as polyethylene, ethylene dichloride, ethylene oxide, ethyl benzene, ethyl alcohol and vinyl acetate. Ethylene is commercially produced by thermal steam cracking (pyrolysis) of hydrocarbons. The Oxidative

dehydrogenation of ethane (ODHE) for the gas phase reaction has been investigated, both experimentally and through kinetic modeling and simulations, as a potential alternative to steam cracking for the ethylene production.

The main objective was to obtain the optimized ethylene yield for the gas phase ODHE. The experiments were carried out at isothermal condition and atmospheric pressure by using a quartz tube flow reactor (2 mm i.d.) with a volume of 0.110 ml. A gas phase kinetic model with 134 elementary reaction steps and 25 species was adopted from literature and the parameters were adjusted by best fitting of the experimental data based on the sensitivity analysis of the kinetic model. Further the model was reduced based on the contribution analysis and a kinetic model of 41 steps involving 23 gas phase species was finally established.

The model predictions were in good agreement with the experimental data for ethane conversion and product selectivity. The gas phase ODHE reaction was further analysed by means of the established kinetic model for ODHE, by using the one-dimensional plug flow reactor model at isothermal condition. The upper bound of ethylene yield for the gas phase ODHE has been investigated by studying the ethylene yield as a function of ethane conversion at different conditions (such as C_2H_6/O_2 ratio and temperature). For isothermal operations (1173 K), the gas phase ODHE gives ethylene yield of 53.5% at high conversion level (81.9%) and residence time of 0.1 s. The reaction pathways leading to different product formation can, approximately, be analysed on the basis of the activation energy but the radical concentrations influence the rate of each step significantly. Therefore in the present work, we analysed the reaction pathways at the given conditions on the basis of the information collected through rate of production (ROP) analysis. The analysis of ROP is a useful tool for a better understanding of the reacting flow calculations. By this analysis the contribution of each reaction to the net production or destruction rates of a species were determined.

The gas phase ODHE to ethylene for auto-thermal operations have been studied further by, both one-dimensional and two-dimensional, reactor simulations at constant atmospheric pressure. The effect of oxygen distribution with variation of reactor diameter was studied by the two-dimensional reactor simulations. The simulations were carried out for the uniform distribution of oxygen and the variable distribution of oxygen with an inlet temperature of 1023 K and the overall C_2H_6/O_2 ratio of 3.3. High ethylene yield, for the reactor of bigger diameter (1.0 m), was strongly associated with the uniform distribution of oxygen. On the other hand, the effect of oxygen distribution upon ethylene yield was negligible for the reactor of smaller diameter (0.2 m).

The one-dimensional reactor model was used for the optimization of the ethylene yield with auto-thermal operations. The ethylene yield of 57.8% (C_2H_4 selectivity 70.2%) was predicted for the gas phase ODHE with an inlet temperature of 1023 K and a reactor length of 2 m at atmospheric pressure. The

effect of different conditions, inlet velocity (1-3 m/sec), inlet temperature (1023-1123 K) and C_2H_6/O_2 ratio (2.5-5.0), upon ethylene yield was analyzed. The C_2H_6/O_2 ration of 3.3 and the inlet temperature of 1023 K were found as the best operating conditions for the gas phase ODHE and auto-thermal operations with inlet velocity of 1.58 m/sec at standard condition. The ethylene yield of 57.8% (C_2H_4 selectivity 70.2%) was predicted by using the multiple injections of oxygen feed for the overall C_2H_6/O_2 ration of 3.3 with an inlet temperature of 1023 K and a reactor length of 2 m at atmospheric pressure.

Conversion of synthesis gas from biomass to liquid fuels by the Fischer-Tropsch synthesis

Ph.D. Candidate: Andreas Helland Lillebø
Post.doc: Bjørn Christian Enger
Supervisor: Prof. Anders Holmen
Co-supervisor: Prof. Edd A. Blekkan

The main objective is to study CO hydrogenation (Fischer-Tropsch synthesis) on modified Fischer-Tropsch catalysts using synthesis gas ($CO + H_2$) derived from biomass. The technology for conversion of biomass to liquid fuels (BTL) is similar to the technology for gas to liquids (GTL) and the objective is to focus on the differences and challenges specific to biomass derived synthesis gas. In particular, biomass derived synthesis gas contains large amounts of contaminants like alkali, H_2S, COS, NH_3, HCN, dust and tars. Cobalt based Fischer-Tropsch catalysts are very sensitive to contaminants and ppm levels of contamination is known to modify the hydrocarbon selectivity and cause catalyst deactivation. It is possible with state-of-art technology to remove the contaminants down to acceptable levels. However, the economic risk related to a trip or failure, where a breakthrough of contaminants reaches the catalyst, is very high because of the high replacement cost for the catalyst. Thus, knowing the severity of and managing this risk as well as designing catalysts which are more tolerant to contaminants will help to reduce the commercial risk for BTL.

Publications and presentations in 2012:

1. Bjørn Christian Enger, Anders Holmen, *Review: Nickel and Fischer Tropsch synthesis*, Catalysis Reviews in Science & Engineering 54(4) (2012) 437-488.
2. Bjørn Christian Enger, Rune Lødeng, Anders Holmen, *On the nature of elementary reactions from methane to hydrogen over transition metals*, Int. J. Hyd. Energy 37 (2012) 10418-10424.

3. Bjørn Christian Enger, Anders Holmen, *The cobalt particle size effect in Fischer-Tropsch synthesis: Some perspectives based on statistics and particle size distributions*, poster and presentation at the 15th International Congress on Catalysis (ICC), Munich, Germany, 1-6 July 2012
4. Bjørn Christian Enger, Jia Yang, Anders Holmen, *Reaction mechanisms for CO hydrogenation: Alternative rate limiting steps*, poster presentation at Synfuel 2012 symposium, Munich, Germany, 29-30 June 2012
5. Bjørn Christian Enger, Anders Holmen, *On the nature of Fischer-Tropsch synthesis: thermodynamics and catalysis*, oral presentation at the Nordic Catalysis Symposium (NCS), Mariehamn, Aaland, 9-12 June 2012
6. Andreas Helland Lillebø, Sindre Håvik, Edd Anders Blekkan, Anders Holmen, *SiC as support material for Co-based Fischer-Tropsch catalysts*. 15th Nordic Symposium on Catalysis, Åland, Finland, June 10-12, 2012.
7. Andreas Helland Lillebø, Erling Rytter, Edd Anders Blekkan, Eleni Patanou, Anders Holmen, *Effect of Alkali on Co-based Fischer-Tropsch catalysts*. International Symposium on Alternative Clean Synthetic Fuels (SynFuel 2012); Munchen, Germany June 29 -30, 2012.
8. Edd Anders Blekkan, *Biodrivstoff via gass og Fischer-Tropsch syntese: Katalytiske utfordringer.* Teknologisk møteplass - Bioenergi og biodrivstoff, Norges Forskningsråd, Oslo June 14, 2012.
9. Edd Anders Blekkan, *Biomass to liquid fuels: The gasification route*, Technoport 2012; Trondheim, Norway April 16-18, 2012.
10. Edd Anders Blekkan, *Fra trevirke til diesel*. Transportforskning 2012, Norges Forskningsråd, Oslo September 3, 2012.
11. Vincent Eijsink og Edd A. Blekkan, *Visjoner for Norges bidrag til den globale forskningen på 2. generasjons biodrivstoff.* Bioenergidagene 2012 (NoBIO), Hamar November 5-6, 2012.

Financial support:
The Norwegian Academy of Science and Letters (VISTA), Statoil, SINTEF, NTNU and Norwegian Research Council through NRC project 190763 Biomass to liquid fuels.

New concepts in the catalytic dehydrogenation of propane

Ph.D. Candidate: Ilya V. Gorelkin
Supervisor: Prof. Edd A. Blekkan

The production of light alkenes (C_2-C_4) is a central part of the petrochemical industry. Due to a higher growth in the demand for propene compared to other alkenes, the selective production of propene via catalytic dehydrogenation of propane is interesting. In this project we study fundamental and applied issues in

propane dehydrogenation, mainly the development of a new concept in process heating. The concept is based on the *in situ* catalytic combustion of hydrogen, at conventional processing conditions for propane dehydrogenation, i.e. around 600 °C. The investigations address reactions between hydrogen and oxygen on supported platinum catalysts in the presence of hydrocarbons (propane, propene).

A microkinetic model for this system is under construction, supported by experimental investigations, exploring the effect of catalyst composition and reaction conditions on the yields of products.

Publications in 2012:

1. I.V. Gorelkin, E.A. Blekkan: *Catalytic dehydrogenation of propane coupled with hydrogen combustion studied over a Pt-Sn catalyst using ternary yield plots*. Submitted (Chem. Eng. Journal).
2. I.V. Gorelkin, E.A. Blekkan*: A microkinetic model of the oxygen-assisted dehydrogenation of propane over a supported platinum catalyst*. In preparation.

Financial support:
The Gassmaks program from The Research Council of Norway.

Artificial photosynthesis /Converting sunlight into applicable energy

Ph.D. Candidate: Ida Hjorth
Supervisors: Prof. De Chen, Prof. Magnus Rønning

This project aims to take a step towards realization of "artificial photosynthesis". Artificial photosynthesis can be done by a photo-electrochemical system. It stores the energy from the sun in chemical bonds by photo-catalytic water splitting and possibly also photo catalytic CO_2 reduction. The design of a photo-electrochemical system is demanding. There is an intense search for materials that can efficiently produce solar fuels without sacrificial agents or other energy inputs, and can withstand corrosion. Key problems involve efficient utilization of sunlight by band gap matching and efficient charge separation, and lowering of high activation over potentials by finding a suitable catalyst.

By functionalizing aligned carbon nanotubes with a semiconductor with a proper band gap the separation of excited holes and electrons can be improved. The nano-structuring of the photo-active material may also increase absorption of light due to internal scattering.

An interesting strategy is to functionalize aligned carbon nanotubes with iron oxide as photo-active material and manganese or cobalt oxide clusters as a catalyst for water splitting. The slight mismatch of the conduction band of iron oxide with the redox potential of water can be compensated by an external bias provided by a thermogalvanic cell.
The power source of the thermogalvanic cell may also be the sun itself, by converting light into heat. Aligned carbon nanotubes is "the darkest material" found, meaning it adsorbs nearly all irradiation. The energy of the adsorbed light is converted to heat, and therefore an irradiated electrode consisting of a metal foil with aligned carbon nanotubes on both sides may serve as an excellent hot electrode for a thermogalvanic cell. The front side absorbs sunlight and produces heat, while the back side will have a large interface with an electrolyte. Functionalization of the CNTs by doping or oxidation can improve the kinetics of electron transfer.

So far, I have created a thermoelectric cell based on aligned CNTs on aluminum foil, using aqueous ferrocyanide or TBAN in dodecanol as electrolytes. The aligned tube structure gives a cell with power densities higher than what is published for related thermogalvanic cells.

Presentations/Posters in 2012:

1. Ida Hjorth, De Chen: *Harvesting low grade energy by CNT/electrolyte based thermoelectric cells.* Oral presentation. Annual NanoLab conference, Trondheim December 2012.
2. Ida Hjorth, Fengliu Lou, De Chen: *Energy harvest by thermoelectric cells based on N-doped aligned carbon nanotubes on metal foils.* Poster and presentation. Chemistry for Energy, Berlin, January 2013.

Financial support: Strategic funding, NTNU.

Advanced Catalysis in Methane Decomposition

Ph.D Candidate: Fengliu Lou
Supervisor: Prof. De Chen

The object of this project is to obtain aligned carbon nanotubes on the surface of conductive substrates, clays and grapheme. Also to prepare carbon nanofiber pellets with good mechanical strength and high surface area. And then obtain a microkinetic model that can describe the carbon nanofiber/nanotube formation process.

Aligned carbon nanotubes were synthesized over Al foil, copper foil and stainless steel successfully, and they were used as electrodes for energy storage, such as supercapacitor and lithium ion battery. Carbon nanofibers pellets were prepared by growth carbon nanofibers among the layers of expended graphite as electrode for supercapacitors. The microkinetic model for describing carbon nanotubes growth waits to be developed.

Publications in 2012:

1. F. Huang, F. Lou and D. Chen, *Exploring Aligned-Carbon-Nanotubes@Polyaniline Arrays on Household Al as Supercapacitors*, ChemSusChem, 2012, 5, 888.
2. Fengliu Lou, Haitao Zhou, Fan Huang, Fride Vullum-Bruer, Trung Dung Tran, De Chen, *Facile Synthesis of Manganese Oxide/Aligned Carbon Nanotubes over Aluminium Foil as 3D Binder Free Cathodes for Lithium Ion Batteries*, Journal of Material Chemistry A, 2013, 1, 3757-3767.
3. Fengliu Lou, Haitao Zhou, Fride Vullum-Bruer, Trung Dung Tran, De Chen, *Synthesis of carbon nanofibers@MnO2 3D structures over copper foil as binder free anodes for lithium ion batteries*, Journal of Energy Chemistry, 2013, 22, 78-86.
4. Haitao Zhou, Fengliu Lou, Per Erik Vullum, Mari-Ann Einarsrud1, De Chen, Fride Vullum-Bruer, *3D Aligned-Carbon-Nanotubes@ Li2FeSiO4 arrays as high rate capability cathodes for Li-ion batteries*, Nanotechnology, submitted.
5. Fengliu Lou, Haitao Zhou, Trung Dung Tran, Marthe Emelie Melandsø Buan, Fride Vullum-Bruer, Magnus Rønning, John Charles Walmsley and De Chen, *Coaxial carbon/MnOx/aligned carbon nanotubes arrays over stainless steel foil as binder free anodes for lithium ion batteries*, Journal of material chemistry A, submitted.
6. Fengliu Lou, De Chen, *Aligned carbon nanotubes based 3D electrodes for high power electrochemcial energy storage application*, in preparation.
7. Fengliu Lou, De Chen, *Facile and Scalable Synthesis of Activated Carbon Nanofibers/Graphene Nanosheet Hybrids for High Performance Supercapacitors*, in preparation.
8. Fengliu Lou, Haitao Zhou, Fan Huang, Fride Vullum, De Chen, *Synthesis of MnO2/Aligned Carbon Nanotubes/Aluminum Foil 3D Nanomaterials as Binder Free Cathode for lithium ion batteries*, Oral presentation, Annual World Conference on Carbon 2012, Krakow, Poland

Doped carbon nanomaterials as metal-free catalyst

Postdoctoral Fellow: Navaneethan Muthuswamy
Supervisor: Prof. Magnus Rønning
Co-supervisor: Prof. De Chen

The project deals with rational design of carbon-based nanomaterials to replace the traditional platinum-based catalysts used for oxygen reduction reaction (ORR) in fuel cell technology and oxidative dehydrogenation (ODH) reaction in production of light olefins. Carrying out the ORR with carbon nanostructures, could replace the noble metals used in certain applications like DMFC (direct methanol fuel cells) and PEMFC (polymer electrolyte membrane fuel cells). Current ODH catalysts do not possess sufficient activity and selectivity; the latter due to the catalyst's inability to prevent complete substrate oxidation. The currently used catalysts are either based on vanadium or Pt. Vanadium based catalysts are highly selective, but their activity is relatively low. On the contrary, Pt-based catalysts are more active, but with scarce selectivity.

For both reactions, ORR and ODH, chemisorption and dissociation of the O_2 molecule on carbon nanomaterials plays an important role, and can be tuned by modifying the electronic properties of the carbon nanomaterials through doping impurities such as N, B, P etc. In the first phase, the project will be focused on N-doped carbon nanostructures for ORR. The samples will be prepared at different synthesis conditions and tested for ORR in oxygen saturated electrolytes. The intermediates at the electrode surface (formed during oxygen reduction) that facilitating the oxygen reduction will be elucidated and correlated with the X-ray photoelectron spectroscopy (XPS), Fourier transform infrared spectroscopy (FTIR), Raman spectroscopy, temperature programmed oxidation (TPO) and cyclic voltammetry results.

Publications in 2012:

1. Navaneethan Muthuswamy, Jose Luis Gomez de la Fuente, Piotr Ochal, Rajiv Giri, Steinar Raaen, Svein Sunde, Magnus Rønning and De Chen, *Towards a highly-efficient fuel-cell catalyst: optimization of Pt particle size, supports and surface-oxygen group concentration*, Phys. Chem. Chem. Phys, DOI: 10.1039/c3cp43659d
2. Navaneethan Muthuswamy, Jose Luis Gomez de la Fuente, Dung T. Tran, John Walmsley, Mikhail Tsypkin, Steinar Raaen, Svein Sunde, Magnus Rønning, De Chen, *Ru@Pt core-shell nanoparticles for methanol fuel cell catalyst: Control and effects of shell composition*, Accepted in Int. J. Hydrogen Energy

Financial support:
The project is funded by the European Union 7th Framework Programme (NMP-FP7) through the FREECATS project.

Sorption Enhanced High Temperature Water Gas Shift Reaction: Materials and Catalysis

Ph.D. Candidate: Tayyaba Noor
Supervisor: Prof. De Chen

Steam reforming is currently the major process for large-scale production of hydrogen. Hydrogen production from steam reforming is a process that involves multiple steps and severe operating conditions. A pre-reforming step is normally necessary to convert heavy hydrocarbons to methane and synthesis gas, in order to lower the coking potential. The reformer is followed by high and low temperature water-gas shift reactors, and then carbon dioxide removal. The hydrogen production by high temperature water gas shift reaction in conjunction to reforming process, as a significant industrial method for hydrogen generation has been studied. The work is directed towards synthesis of catalyst and sorbent materials, evaluation for kinetic parameters and reaction mechanism, and sorption enhanced study to produce fuel cell grade hydrogen focusing high temperature water gas shift reaction. The main objective has been to achieve hydrogen rich product stream for fuel cell purpose and to screen a better catalyst for this purpose.

Publications in 2012:

1. T. Noor, A. Lind, A. Holmen, D. Chen, *Synthesis of micro-spherical hydrotalcite derived Ni-Co bimetallic catalyst using spray drying method*, in preparation.
2. T. Noor, J. Zhu, D. Chen, *High temperature water gas shift reaction over bimetallic Ni-Co catalyst: Mechanism and Kinetics*, in preparation.
3. T. Noor, M. V. Gil, D. Chen, *Production of fuel-cell grade hydrogen by sorption enhanced water gas shift reaction using Pd/Ni-Co catalyst*, in preparation.

Presentations in 2012:

1. T. Noor, S. S. Kazi, D. Chen, *Development and testing of mix oxide nanoparticles for CO_2 capture in sorption enhanced reactions*, InGAP NANOCAT Summer School, Trondheim Norway. June 21-26, 2009 (Poster).

2. T. Noor, A. Lind, A. Holmen, D. Chen, *Synthesis and characterization of Ni hydrotalcite catalyst for hydrogen production using co- precipitation, spray drying and micro-emulsion method*, Norwegian Symposium on Catalysis, Trondheim Norway, November 30- December 1, 2009 (Poster).
3. T. Noor, A. Lind, A. Holmen, D. Chen, *Integrated process for hydrogen production with CO_2 capture using sorption enhanced reforming reactions,* 9th Natural gas conversion Conference, Lyon, France, May 30- June 3, 2010 (Poster).

Financial Support:
The project is funded by Norwegian Research Council through KOSK Programme.

New approach to metal dusting corrosion

Ph.D. Candidate: Daham Sanjaya Gunawardana Panditha-Vidana
Supervisors: Prof. Hilde Venvik and Prof. De Chen

Metal dusting is a catastrophic corrosive degradation process on metals and alloys that proceeds by a gradual breakdown of materials into fine dust like particles. It constitutes a problem in the chemical and petrochemical industries, where metals and alloys are exposed to carbon-supersaturated gaseous environment with low oxygen or steam partial pressures (carbon activity, $a_{c>1}$) at temperatures above 400^{o}C. Metal dusting carries significant cost associated with precautionary measures and, ultimately, replacement of certain process unit and equipment.

The overall objective of this study is to obtain better understanding of the initial stages in metal dusting corrosion, i.e. the initiation of the carbon formation. This is done by differently preparing surface oxide layers of a representative alloy, which is then exposed to high carbon activity (a_C>1) gas atmosphere at high temperature. This is combined with detailed characterization before and after the exposure in order to find a relationship between the structure and composition of the alloy, the oxide layer and its propensity to form solid carbon. Since the initial carbon formation as well as the progress of the metal dusting is affected by numerous parameters, including even the flow pattern and material stress as well as the more obvious structure and composition of the exposed alloy surface, temperature, pressure, and composition of the gas stream, great care has been taken to choose consistent experimental procedures that treat one parameter at the time.

The Ni-based industrial alloy (Inconel 601) samples have first undergone oxidation treatment and then been subjected to CO exposure. Oxidized as well as CO exposed samples were examined in optical microscopy, SEM and

combined depth profiling by ion-sputtering and AES. Results showed that the increasing pre-oxidation temperature was found to create a surface oxide layer with better resistance to carbon formation under CO exposure treatment, irrespective of the oxygen partial pressure in the pre-treatment gas and the initial sample preparation (as-received vs. polished). But the extent of carbon formation on sample surface is governed by the parameters of the preceding oxidation as well as the method of sample preparation. The higher carbon formation on the samples pre-treated at low temperature is attributed to the Ni and/or Fe rich surface oxide layer compare to their high temperature counterparts. Higher the oxidation temperatures deplete the presence of Ni and Fe species in the surface oxide layer and saturate the thick oxide layer with Cr. Carbon formed on the samples is also investigated by means of TEM. It reveals that Ni rich metal particles are associated with carbon filaments.

Presentations and publications in 2012:

1. P.V.D.S. Gunawardana, J. Walmsley, A. Holmen, D. Chen, H.J. Venvik. *Metal dusting corrosion initiation in conversion of natural gas to synthesis gas*, Energy Procedia 26, 125–134 (2012).
2. P.V.D.S. Gunawardana, J. Walmsley, H.J. Venvik: *Study of the initiation of metal dusting corrosion*, Oral presentation in inGAP seminar; Oslo, Norway: 6–7th December, 2012.
3. P.V.D.S. Gunawardana, J. Walmsley, D. Chen, A. Holmen, H.J. Venvik: *Investigation of metal dusting corrosion initiation in natural gas conversion,* Poster presentation in SynFuel 2012 Symposium; Munich, Germany: 29–30th June, 2012.
4. P.V.D.S. Gunawardana, J. Walmsley, D. Chen, A. Holmen, H.J. Venvik: *Investigation of metal dusting corrosion initiation in natural gas conversion*, Poster presentation in The 15th Nordic Symposium on Catalysis; Mariehamn, Åland, Finland: 10–12th June, 2012.

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Microcalorimetry and microkinetics of heterogeneous catalysts.

Ph. D Candidate: Eleni Patanou
Supervisor: Prof. Edd A. Blekkan
Co-supervisor: Prof. De Chen

Adsorption of the reactants is the first step in a sequence of dynamic phenomena occurring on a catalytically active surface. The adsorption of reactants involves the exchange of energy due to bond breaking and forming processes, therefore the accurate determination of the heat of adsorption of reactants is of high relevance in catalysis. The most reliable method that facilitates the determination of the energy of the bonds between the adsorbed species and the adsorbents is adsorption calorimetry. The technique allows accurate determination of the strength of surface sites by the direct measurement of the heat of adsorption of suitable probe molecules. The improved sensitivity of modern calorimeters and the development of refined data analysis techniques have made adsorption microcalorimetry a tool of significant contribution to the characterization of catalytic surfaces. The acquired information on surface energetics can be used as input to microkinetic models that are constructed based on binding energies of molecules on the surface, for predicting catalyst performance. A modern approach of improving and developing heterogeneous catalysts is based in such a link of information from theory and surface science in order to improve the catalyst design and the optimization of catalytic processes.

In the present work the adsorption microcalorimetry method and a microcalorimetric apparatus were established in order to obtain the heats of adsorption of different probes on real catalytic surfaces. Catalysts were chosen from a process with high industrial significance, the Fischer-Tropsch synthesis. To enable the pre-treatment of metal supported catalyst in the metallic state and to preserve it during analysis a homemade microcalorimetric flow cell was constructed. The surface response of activated cobalt supported Fischer-Tropsch synthesis catalysts was measured for the key probe molecules of H_2 and CO. The structure sensitive character of the reaction and the effect of the alkali metals addition on Fischer-Tropsch catalysts were investigated in detail. An attempt to correlate adsorption enthalpies with observed differences on the activity and selectivity of these materials was done. The results indicated that Co nanoparticles exhibit a high heterogeneity exhibiting two different adsorption energy regimes; however only minor differences were detected between the catalysts materials by adsorption microcalorimetry in the examined range. Alkali addition on the γ-Al_2O_3 supported cobalt catalyst did not affect the heat of adsorption, when ppm amounts were added, while some differences were observed when the loading was increased to 1 and 2 wt% Na. The enforced

bonding attributed to the charge transfer from Na onto neighboring Co sites could be detected only for the catalysts samples containing high loading of Na added. In all cases the CO appears to adsorb stronger than H_2, giving higher heat of adsorptions.

Publications in 2012:

1. E. Patanou, E. Z. Tveten, D. Chen, A. Holmen, E. A. Blekkan*: Microcalorimetric studies of H_2 and CO on Co/γ-Al_2O_3 catalysts for Fischer –Tropsch synthesis*. In press, Catalysis Today. (http://dx.doi.org/10.1016/j.cattod.2012.12.006)
2. E. Patanou, A. Lillebø, De Chen, A. Holmen, E.A. Blekkan: *The effect of alkali metals on Cobalt based Fischer-Tropsch catalysts*. Submitted Catalysis Today.
3. Eleni Patanou: *Adsorption microcalorimetry studies on supported cobalt catalysts*. PhD-thesis, Doctoral theses at NTNU, 2012:247.

Presentations in 2012:

1. E. Patanou, De Chen, E. A. Blekkan: *Adsorption of H_2 and CO on cobalt supported catalysts for the FT synthesis studied by microcalorimetry – effect of cobalt particle size*. Poster presentation, 15th ICC, 1-4 July, Munich, Germany 2012.
2. E. Patanou, De Chen, E. A. Blekkan: *Microcalorimetric studies of H_2 and CO supported catalysts for Fischer – Tropsch synthesis*. Oral presentation, Syngas Convention, 1 - 4 April, Cape Town, South Africa 2012.
3. E. Patanou, E.A. Blekkan: *Adsorption microcalorimetry*. Oral presentation, inGAP seminar, Univ. of Oslo, Dec. 6-7, 2012.

DFT Studies on mechanisms of Fischer-Tropsch synthesis

Ph.D. Candidate: Yanying Qi
Supervisors: Prof. De Chen and Prof. Koch Henrik

The increase in the demand for transportation fuels and newly discovered huge reserves of coal and natural gas has made F-T synthesis more attractive as a promising alternative route to produce liquid fuel. Detailed reaction mechanisms and kinetic analysis could provide principles for rational design of F-T catalysts to achieve better activity, selectivity and stability. Because of competitive reaction routes and complex catalyst surface structure, although the reaction

mechanisms were explored by numerous experiments and theoretical calculations, it is still a project of immense controversy and uncertainty.

With the advent of sophisticated computational chemistry techniques, the intricate electronic-structure calculations based on density functional theory (DFT) are widely used to provide vital fundamental information which is difficult to obtain by experimental methods. It could provide important data regarding the transition states, intermediates, activation energy of each elementary step involved in F-T reactions. To provide deeper insight to the fundamental mechanisms, DFT has been widely used in the F-T synthesis research. Combined experimental and DFT investigation of kinetic isotope effects (KIE) will serve as versatile tools to elucidate reaction mechanisms and the nature of transition states.

The objective of the present work is to establish a comprehensive microkinetic model of F-T synthesis on Co catalysts including CO activation and chain growth, which will be achieved by national and international cooperation. DFT calculations and kinetic isotope effect analysis will be combined to elucidate details regarding the reaction mechanism and rate determining steps of CO dissociation.

Financial support:
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Dehydrogenation of NGL components at very short contact times

Ph.D. Candidate: Paul B. Radstake
Supervisor: Prof. Anders Holmen
Co-supervisor: Prof. Magnus Rønning

Lower olefins such as ethene and propene are important intermediates for a large number of industrial processes. NGL (C_2-C_4 components in natural gas) is an excellent feedstock for production of lower olefins and Norway has access to large quantities of NGL. Oxidative dehydrogenation at very short contact times represents a new, exciting and promising way of converting NGL components to the corresponding olefins. It holds the promise of greatly reducing the reactor volume, as well as of autothermal operation. Another advantage is that it overcomes the thermodynamic limitations and avoids the necessity of continuous catalyst regeneration.

The purpose of the project is to characterize the oxidative dehydrogenation of NGL components at very short contact times and high temperatures. The focus of the project is mainly on the selection of both convenient catalytic systems and suitable characterization techniques in order to

further understand the fundamentals of this type of reactions. The experimental work is based on powdered Pt-Sn catalysts. Parameters to be investigated are mainly catalyst loading, atomic ratios of the different elements, type of support, synthesis procedures and catalyst precursors. The characterization is based on both physicochemical and spectroscopic techniques as well as the catalytic performance. Parameters within the catalytic testing experiments are investigated as well. These parameters include reaction temperature, gas flow rates and gas ratios.

Publications:

1. P.B. Radstake, M. Rønning, A. Holmen: *Platinum-tin catalysts: A short review*. In preparation.
2. P.B. Radstake, M. Rønning, A. Holmen: *Influence of H_2 on the oxygen-assisted dehydrogenation of ethane over Al_2O_3-supported Pt-Sn catalysts.* In preparation.
3. P.B. Radstake, M. Rønning, A. Holmen: *The effects of complete O_2 conversion during oxygen-assisted dehydrogenation of ethane over Al_2O_3-supported Pt-Sn catalysts.* In preparation.
4. P.B. Radstake: *Oxygen-Assisted Dehydrogenation of Ethane over Al_2O_3-Supported Pt-Sn Catalysts.* Doctoral theses at NTNU, 2012:376.
5. P.B. Radstake, M. Rønning, A. Holmen: *Oxygen-Assisted Dehydrogenation of Ethane over Pt-Sn Catalys.* Accepted as an oral presentation at EuroCat2013 in Lyon.

Financial support:
The project is funded by the Norwegian Research Council (NFR), through the GASSMAKS program.

Model systems for Co – based Fischer -Tropsch catalysts

Ph.D. Candidate: Marie Døvre Strømsheim
Supervisor: Prof. Hilde J. Venvik
Co-supervisor: Prof. Anne Borg

The motivation behind this research is to explore the surface chemistry of adsorbates on model Co surfaces in the context of the Fischer Tropsch synthesis (FTS). Cobalt is often preferred in modern, natural gas based FTS technology, but despite this there has to date been relatively few studies on model Co surfaces. Performing surface science studies of this model system with relevant reactants such as CO/H_2 (syngas) as well as well as possible catalyst poisons,

can elucidate important aspects of adsorption and reactions at the surface. This can provide insight into what occurs at the surface of a real FT-catalyst.

Structural and chemical characterization will be carried out on Co single crystals, such as Co(0001), Co(11-20), Co(10-10) and Co(10-12). The overall structure of the surface and degree of ordering of the sample will be determined by low energy electron diffraction (LEED). The surface geometry, sites of adsorbates and local structural changes as a result of adsorbates and reactions occurring at the surface will be studied with scanning tunneling microscopy (STM). Since STM mainly provides information regarding structure the chemical characterization of the model systems in question will be performed with X-ray photoelectron spectroscopy (XPS). This technique can provide chemically specific core level energies of the electrons in the top layers of the surface. Near ambient pressure XPS (AP-XPS) with pressures up to ~25 mbar, will be performed at the synchrotron facilities in Lund, Sweden, in order to obtain results at conditions closer to the elevated temperatures (200-230°C) and pressures (>20 bar) which are applied for industrial FT-catalysts.

Financial support
This project is funded by the Research Council of Norway (NFR) and NTNU, through the Innovative Natural Gas Processes and Products program (inGAP).

Understanding catalytic effects in Pd alloy model systems and membranes through advanced characterization and modelling.

Postdoctoral Fellow: Ingeborg-Helene Svenum
Supervisors: Professor Hilde J. Venvik, Professor Manos Mavrikakis, Univ. of Wisconsin-Madison, USA, Professor Anne Borg, Dept. of Physics, NTNU

The manipulation of adsorption properties of catalysts and membranes in H_2/CO mixtures has been targeted by many researchers, and has relevance to natural gas conversion in general and hydrogen technology in particular. We discovered that CO inhibition of hydrogen transport through PdAg membranes was significantly reduced by membrane heat treatment in air. Analysis indicated changes in CO an H_2 heats of adsorption to play a role and surface spectroscopy indicated segregation phenomena to be involved. The overall objective of the project is therefore to understand the response of Pd alloy surfaces to carbon monoxide and carbon dioxide the in presence of hydrogen by advanced characterization techniques in conjunction with detailed calculations, and to apply this knowledge to improved membranes, membrane reactors and catalysts.

Using periodic self-consistent density functional theory (DFT) calculations, we have investigated the H_2/CO/O_2 adsorbate system over a

$Pd_3Ag(111)$ model system in order to better understand the effect of a reactive environment on surface segregation behaviour. Our DFT calculations showed that the $Pd_3Ag(111)$ surface is rich in Ag under UHV conditions in agreement with the literature. In the presence of O, H, and CO adsorbates, however, Pd atoms are pulled to the topmost surface layer, making the $Pd_3Ag(111)$ surface Pd-dominated at the corresponding saturation coverages. The DFT studies further indicate that segregation within the uppermost layers of a $Pd_3Ag(111)$ surface may affect hydrogen adsorption, and hence possibly the overall hydrogen transport through the membrane. CO poisoning is a common problem for Pd-based membranes. Preliminary results indicate that the surface composition and CO coverage influence the activation of H_2

The project partners are the NTNU Departments of Chemical Engineering and Physics and SINTEF Materials and Chemistry, with the University of Wisconsin-Madison as an international partner. The research is conducted through the postdoctoral fellowship and one PhD project at Dept. of Physics. Experimental investigations of binding energies, adsorption sites and surface species are targeted through modelling and experiments. The density functional theory calculations are performed using the DACAPO code, which is a state-of-the-art plane wave-pseudopotential implementation of DFT. Characterization is performed through high resolution, surface sensitive photoelectron spectroscopy and diffraction using high intensity, X-ray range, tuneable synchrotron radiation. Both model systems (single crystals) and membrane samples surfaces (sputtered Pd alloy thin films) are being studied.

Publications and presentations in 2012:

1. I.-H. Svenum, J.A. Herron, M. Mavrikakis, H.J. Venvik, *Adsorbate-induced segregation in a PdAg membrane model system: $Pd_3Ag(111)$*, Catalysis Today, 193 (2012) 111.
2. 12th International Conference on Inorganic Membranes, Enschede, The Netherlands, 9 – 13 July, 2012. *Co-adsorption of H and CO on a Pd-Ag membrane model system: Pd3Ag(111)*, oral presentation.
3. 14th International Conference on Theoretical Aspects of Catalysis, Vlissingen, The Netherlands, 26 – 30 June, 2012. *Adsorbate-induced segregation and coadsorption on a Pd-Ag membrane model system*, oral poster presentation.
4. 15th Nordic Symposium on Catalysis, Mariehamn, Åland, 10 – 12 July, 2012. *Co-adsorption of hydrogen and carbon monoxide on Pd3Ag(111)*, oral presentation.
5. Seminar in connection with the appointment of Professor Jens Nørskov, Stanford University as a Honorary Doctor at NTNU, 31 May, 2012. *Modeling of adsorption on Pd3Ag alloy surfaces*, oral presentation.

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The project is funded by the Research Council of Norway (KOSK II programme, Contract No. 197709/V30) and Statoil ASA through the NTNU-SINTEF Gas Technology Centre.

Insulating liquids

Ph.D. Candidate: Ingvild Tronstad
Supervisors: Prof. Edd A. Blekkan, Dr. Marit-Helen G. Ese, SINTEF Energiforskning AS.

High voltage transformers are insulated with mineral oil and solid cellulose (paper wrapped around the copper windings). Failures (short-circuits), caused by deposits on the windings in these transformers have dramatic consequences for everyday life and industry. To prevent failures it is important to understand how the insulating materials work in the transformer. By the use of traditional analytical methods such as titration, as well as introducing new techniques such as QCM (Quartz Crystal Microbalance) and microcalorimetry, we try to understand the reactions and effects of the chemicals in the insulating materials. Corrosion and formation of copper sulfide in transformer insulations and oxidation of insulating liquids (including alternative, environmentally friendly liquids), are the main areas of study. The project is a part of the KMB project Thermal and electromagnetic performance of transformers, which is a joint effort between NTNU, SINTEF Energiforskning AS, Statnett, Hafslund, Statkraft, EDF, ABB, Nynäs, Siemens, NVE and The Research Council of Norway.

Publications and presentations in 2012:

1. I. Tronstad, E.A. Blekkan, M.-H. Ese: *Isothermal microcalorimetry as a tool for studying oxidation stability of insulating liquids.* IEEE Transactions on Dielectrics and Electrical Insulation 19(5) (2012) 1528-1536.
2. Ingvild Tronstad, Marit-Helen G. Ese, Edd A. Blekkan: *A Study of the Effect of Copper and Additives in Hydrocarbon and Ester Based Insulating Liquids with Isothermal Microcalorimetry*. Submitted, IEEE Transactions on dielectrics and electrical insulations.
3. Ingvild Tronstad, Carl Marius Roel, Wilhelm R. Glomm, Marit-Helen G. Ese, Edd A. Blekkan: *Ageing and Corrosion of Paper Insulated Copper*

Windings: The Effect of Irgamet39 in Aged Insulated Oil. Submitted, IEEE Transactions on dielectrics and electrical insulations.

Financial support:
Statnett, Hafslund, Statkraft, EDF, ABB, Nynäs, Siemens, NVE and The Research Council of Norway.

Photocatalytic fuel production by reforming of hydrocarbons and CO_2

Ph.D. Candidate: Punchi Patabandige Charitha Udani

Supervisor: Professor Magnus Rønning

The photocatalytic fuel production using solar energy is a challenging research topic which has received much attention in recent years for its potential to provide H_2 as a clean and renewable energy carrier even on a large scale. This can be done with the use of several methods including water photosplitting and even more efficiently, by photoreforming of organic compounds, including methane, alcohols, aldehydes and organic acids to yield H_2 and CO_2 mixtures. The increasing levels of CO_2 in the atmosphere have now become a global environmental issue because of the greenhouse effect. There have been various approaches not only for recycling of this greenhouse gas but also for an efficient production of fuel alternatives. It is reported that CO_2 can be re-introduced in the energy cycle by photoreforming into fuels such as CO, CH_4, CH_3OH, and H_2 .

The project is mainly focused on producing fuel alternatives with the use of an artificial solar light source and various photocatalysts. Various hydrocarbons, catalyst synthesis methods and catalysts formulation will be used, comparing noble metals with transition metals and combinations of these with the aim to prepare cost-effective catalyst systems. To investigate the crystal phase changes and morphology changes, the photocatalysts will be subjected to characterization also after exposure to the reaction conditions and as far as possible, in situ characterization when the catalysts are working.

Financial support:
The project is funded by strategic funding, NTNU.

Palladium based membranes in catalytic reactions

Ph.D. Candidate: Nicla Vicinanza

Supervisors: Professor Hilde Johnsen Venvik, Dr. Scient. Rune Bredesen and Dr. Thijs Peters, SINTEF

Palladium-based membranes have been for decades the focus of many studies due to their high hydrogen permeability and selectivity and because they are potential candidates for use in membrane reactors. As palladium is expensive, the main disadvantage that these membranes have is high cost of the material, and the material costs are proportional to the thickness. Reduced thickness also increases the total hydrogen flux through the membrane since hydrogen permeation and palladium thickness generally are inversely proportional. Therefore, the main objective of the recent studies has been focused on the reduction of the thickness of the palladium layer and the improvement of hydrogen permeability. SINTEF has developed a technology to produce palladium alloy membranes with thickness down to 1-2μm that significantly improves flux and reduces material costs. The main aim of this project is to develop thin Pd-alloy membranes with improved thermal stability, sulphur resistance and resistance to flux inhibition by CO, and their integration in reactors and process for water-gas shift and steam reforming.

The basic properties affecting permeation were investigated for membranes in the thickness range from 2.2μm to 10μm, in order to relate the growth structure to the properties. The effect of heat treatment in air (oxidation) was also studied. AFM was applied for structural characterization (topography) of the feed and permeate sides of both treated and as-grown membranes. Sieverts constant (solubility) was obtained from volumetric sorption. The permeation behavior was obtained as a function of temperature and pressure feeding only pure hydrogen with no use of sweep gas and the membrane mounted in a microchannel configuration, in order to have well-defined conditions free of gas phase transport limitations. The results indicate interesting relations between grain structure and solubility, as well as changes over time due to hydrogen permeation and/or heat treatment in air.

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The role of carbon in catalytic dehydrogenation of propane

Ph.D. Candidate: Andrey S. Volynkin
Supervisors: Prof. Edd A. Blekkan, Prof. Magnus Rønning

Carbon can play different roles in catalytic dehydrogenation (DH) of light hydrocarbons. While coke deposition deactivates dehydrogenation catalysts, carbon (with oxygen containing functional groups) can also be catalyst on its own for other dehydrogenation reactions. Another aspect of carbon in dehydrogenation is studies of carbon as support for the active metal. Oxygen containing sites can anchor metal nanoparticles and therefore assist the deposition of metal on carbon. Subsequent reduction in H_2 atmosphere removes the oxygen containing sites and reduces the active metal, making the catalyst able to dehydrogenate hydrocarbons. Metal-support interaction is an important parameter in catalysis and the way Pt and Pt-Sn will interact with carbon support (graphite, active carbon, carbon nanofibres and carbon nanotubes) and the implication of this interaction on the selectivity for DH can be difficult to predict. Carbon nanofibres and carbon nanotubes are not practical catalysts for dehydrogenation-reactions, but provide interesting properties as model systems. The aim of this project is to improve understanding of effects of carbon on catalytic dehydrogenation of light alkanes, especially:

Part of the work in 2012 (October – December) has been performed as a visitor(ASV) with the catalysis group led by prof. Lynn Gladden at the Department of Chemical Engineering and Biotechnology at University of Cambridge, UK.

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Study of the deactivation mechanisms on Co-based Fischer-Tropsch catalysts under realistic working conditions

Ph.D. Candidate: Alexey Voronov
Supervisor: Prof. Magnus Rønning

The Fisher-Tropsch (FT) synthesis is the central step in gas-to-liquid (GTL) technology where H_2 and CO is converted into synthetic crude oil. The hydrocarbons produced in this step are paraffins and olefins with different carbon chain lengths. Due to low water-gas-shift activity, supported cobalt catalysts are often selected as functional materials for the FT synthesis from natural gas.

Since there is no direct method to monitor the behaviour of the Co particles on the support surface, it is essential to apply several characterization techniques in order to distinguish the influence of the various external conditions and define the individual deactivation mechanisms. Investigation at realistic working conditions is necessary to obtain reliable data about the processes which occur on the catalyst during FT reaction. Many parameters have a serious influence to the FT catalyst deactivation, so it is essential to involve several characterization techniques in order to distinguish influence of the various external conditions and define the separate deactivation routes.

Modulation excitation spectroscopy (MES) is a group of techniques which allows us to detect and monitor the dynamic behavior of species involved in a chemical reaction. In combination with suitable in situ spectroscopic techniques it becomes a powerful tool for studying catalytic reactions and investigating catalysts under realistic working conditions.

The MES technique was coupled with X-ray absorption spectroscopy (XAS) in order to investigate catalyst behavior in the FT reaction. A quartz capillary microreactor was used as a micro catalytic fix-bed reactor. Several gases and gas mixtures were exposed to the sample. We have obtained detailed information about surface behavior on a cobalt FT catalyst during red-ox treatment, CO exposure, and also FT synthesis.

The purpose of the project is to obtain detailed information about deactivation mechanisms and the effect of reaction conditions which may lead to new insight in catalyst formulation for FT synthesis in commercial GTL technology.

Financial support:
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The State of Promotors in Fischer-Tropsch Catalysts

Ph.D. Candidate: Georg Voss
Supervisor: Prof. Magnus Rønning

Supported cobalt catalysts are widely studied because of their ability to convert synthesis gas in low temperature Fischer-Tropsch (FT) synthesis. These catalysts provide high activity, high selectivity to long chain paraffins and low water-gas shift activity. It is common practice to add a noble metal promoter to optimize the performance of the catalysts. Recently, more attention has been directed towards a fundamental understanding of the promotion. This study approaches from two perspectives: i) the nature and location of the promotor itself is unclear, especially at reaction conditions, which leads to the utilization

of *in situ* techniques; ii) to mask out pore-size effects and enhance spectroscopic methods, ordered mesoporous alumina is employed as model support for Co Fischer-Tropsch catalysts.

The catalytic behavior of Re and Ni promoted Co-FT catalysts is investigated using modulation excitation spectroscopy (MES) combined with *in situ* X-ray absorption spectroscopy (XAS). MES allows for sensitive and selective detection and monitoring of the dynamic behavior of species directly involved in the reaction. For the purpose of FT *in situ* spectroscopy a setup has be engineered which is capable of performing the experiments at industrially relevant FT conditions (20 bar, 210°C, H_2/CO atmosphere).

Ordered mesoporous alumina as support for FT catalyst provides highly interesting model systems and new opportunities. Being able to control a uniform pore size within the support helps to mask out pore-size effects and opens new possibilities for X-ray diffraction/scattering studies, as the material possess a unique axis.

Finally, this new strategies to reveal the state of promotors in FT catalysts are complimented by *in situ* techniques such as X-ray diffraction (XRD) and small angle X-ray scattering (SAXS) to get information about crystallinity and shape of the particles; as well as a wide range of *ex situ* spectroscopy, scattering, imaging and adsorption techniques, which are used mainly to characterize the status quo of the given system in reference to the promotor.

Publications and presentations in 2012:

1. Norwegian Synchrotron and Neutron User Meeting 2012**,** Stavanger, Norway. Presentation: *The State of Promotors in Fischer-Tropsch Catalysts.*
2. Syngas Convention 2012, Cape Town, South Africa. Presentation: *The State of Promotors in Cobalt Fischer-Tropsch Catalysts.*

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Fundamental study of cobalt-based Fischer Tropsch catalysts using SSITKA

Ph.D. Candidate: Michael Markus Wycisk
Supervisor: Prof. De Chen

The Fischer Tropsch synthesis is a catalytic process that converts synthesis gas to long chain hydrocarbons. This enables the production of high quality diesel petrochemicals from natural gas or biomass. However, even if the process is

already industrialized and working catalysts are available, the mechanism of the process is still under discussion.
Steady-state isotopic transient kinetic analysis (SSITKA) is a powerful method to investigate the mechanism of CO activation and methane formation, by studying the transient response of a switch from $12CO/H_2$ to $13CO/H_2$ syngas under reaction conditions using a mass spectrometer. This allows us to get parameters like the adsorption equilibrium of the adsorbed CO, the site coverage of CO and carbon pools, the reactivity of adsorbed CO, surface resident times of CO and CH_4, the number of surface intermediates and other parameters.
To get accurate results, highly defined catalysts are necessary. Therefore, a new method to synthesize well defined cobalt catalysts should be developed. The project deals with synthesis of colloidal solutions of monodisperse cobalt nanoparticles, following deposition on mesoporous silica like MCF-17 with different pore sizes as supports. A systematic study of activation and selectivity as a function of cobalt nanoparticles sizes in a range of 4 and 20 nm will be performed. A highly integrated approach to combine advanced synthesis and characterization, detailed kinetic study including steady-state and transient, as well as density functional theory is employed to gain a better understanding of the reaction mechanism including CO activation, methane formation and C-C bond formation.
In the second phase of the project, we will study synthesis of Co based bimetallic alloys and core-shell nanoparticles. Those particles should also be supported on mesoporous silica and above approach will be applied to searching for the key factors governing the methane formation and chain growth.

Financial support:
The Norwegian Research Council through the inGAP project (Innovative Natural Gas Processes and Products) and the Department of Chemical Engineering at NTNU.

Steady-State Isotopic Transient Kinetic Analysis (SSITKA) of Catalytic Reactions

Postdoctoral fellow: Jia Yang
Supervisors: Prof. De Chen and Prof. Anders Holmen

Steady-state isotopic transient kinetic analysis (SSITKA) has proved to be a powerful technique for studying heterogeneous catalyzed reactions. By normal steady-state experiments only the overall reaction rate, i.e. the product of the rate constant and the site coverage, is determined. SSITKA combines both the steady-state and the transient technique and makes it possible to study the intrinsic reaction rate at the active catalytic site decoupled from the site

coverage. The method can also be used to study details of the surface reactions such as single or multiple pools of reaction intermediates on the catalytic surface and the reactivity distribution within the pools. A SSITKA experiment consists of making a switch between different isotopic labeled reactant species, such as ^{12}CO and ^{13}CO. The feed for example ^{12}CO-H_2 or ^{13}CO-H_2, is converted at steady-state over the catalyst provided that no isotopic effect occurs, and the transient response after the switch is monitored by a mass spectrometer. The focus so far has been on the production of fuels from natural gas by the Fischer-Tropsch synthesis on Cobalt catalysts. The activity and selectivity depend on the crystal size for small Cobalt particles, and SSITKA has contributed to the detailed understanding of the mechanism.

Recently, the SSITKA transient responses of a switch from ^{12}CO to ^{13}CO have been modeled using a plug flow reactor model. Transient modeling could provide more realistic kinetic parameters for Langmuir-Hinshelwood (L-H) modeling. Combine transient and steady-state modeling (L-H model) could allow detailed mapping of surface species and more insights for the reaction mechanism for CO activation and methane formation in the CO hydrogenation.

Publication and presentations in 2012:

1. Yang, J.; Chen, D.; Holmen, A. *Understanding the kinetics and Re promotion of carbon nanotube supported cobalt catalysts by SSITKA.* Catal Today 2012, 186, 99.
2. J. Yang, D. Chen, and A. Holmen. *New approach for kinetic modeling of Fisher-Tropsch on cobalt based catalysts*. Oral presention.15th International Congress on Catalysis 2012, Munich, Germany, 01-06 July, 2012.
3. J. Yang, J. Zhu, A. Lillebø, D. Chen, A. Holmen. *Effects of interfacial properties of hierarchically structured Co catalysts on Fischer-Tropsch synthesis*. Oral presentation. Synfuel 2012, Munich, Germany, 29-30 June, 2012.

Financial support: The project is funded by the Norwegian research council (NFR), through the "KOSK" program.

Engineering of Pt-based nanoparticles in Propane Dehydrogenation and Co-based nanoparticles in F-T synthesis

Postdoctoral Fellow: Dr. Jun Zhu
Supervisor: Prof. De Chen

Catalytic dehydrogenation of NGL compounds is an important industrial process. Nanocrystals of different size of noble metals are attractive for use as

catalysts because of their different surface-to-volume ratios and high surface area, which in turn cause their surface atoms to be highly active. Meanwhile, nanocrystals of various shape and composition could enable the properties of a nanocrystal to be tuned with a greater versatility than can be achieved otherwise. In this sense, it is of great interest to investigate the effects of Pt and Co surface structure and composition on the dehydrogenation and F-T synthesis reactions.

The project is aimed in that it 1) explores the novel Pt, as well as Co, based nanoparticles with well controlled shapes, sizes and core-shell structures towards catalysts with better activity and good stability, 2) focuses on the fundamental study of the catalyst structure-properties-performance relationship 3) improves the ability in rational design of catalysts in heterogeneous catalysis.

Up to now, 1) Different size and shape of Pt nanoparticles, which have different ratio of surface sites on the surface and varied in the orientations of the surface such as {111}, {100}, have prepared and characterized by XRD, SEM and HRTEM. The effects of surface atoms and facets of Pt nanoparticles on the activity, selectivity and coking in DHP have been investigated for the first time. According to the experimental results, the catalytic performance indicates a strong structure-sensitive character. The reaction mechanism changes with the changing of the different ratio of Pt facets, {111} and {100}, edges and corners exposed on the catalyst surface. DFT simulation data are used to interpret the experimental data and build up dehydrogenation kinetic model. 2) Various core-shell particles, such as Ru@Pt, Ir@Pt, Pd@Pt, Rh@Pt, Ag@Pt, and Co@Pt, have been synthesized and characterized by HRTEM, EDX-line scans, CO-stripping. Different core metals changes the binding energy of propane and hydrogen, so that changes the activity and selectivity of Pt catalysts in DHP. 3) Pt catalysts with small Pt particle size, < 1 nm, encapsulated within NaA zeolite has been prepared. It shows a rather high activity and selectivity in oxidative dehydrogenation reaction. 4) We prepared Co catalysts with Co supported on hierarchically structured carbon nanofibers/carbon felt composites (CNF/CF). With a homogeneous SiO_2 layer on CNF/CF, the oxidation potential of the Co catalyst is lowered, which results in a highly stable catalysts in F-T synthesis.

Publications and presentations in 2012:

1. J. Zhu, A. Holmen, D. Chen. *Carbon nanomaterials in catalysis: proton affinity, chemical and electronic properties and their catalytic consequences*, ChemCatChem, Volume 5, Issue 2, pages 378–401, February 2013
2. J. Zhu, J. Yang, A. H. Lillebø, Y. Zhu, Y. Yu, A. Holmen, D. Chen. *Compact reactor for Fischer-Tropsch synthesis based on hierarchically structured Co catalysts: towards better stability*, Catalysis Today, Accepted
3. J. Zhu, D. Chen, M. Yang, Y. Yu, X. Zhou, A. Holmen. *Selective C-H and C-C Bond Activation of Propane on Platinum Nanoparticles with Different Sizes and Shapes*. Poster presentation in 15th International Congress on Catalysis, Munich, Germany, July 1st to 6th, 2012

4. X. Zhou, J. Zhu, Q. Li, Z. Sui, M. Yang, Y. Zhu, D. Chen, *DFT Based Kinetics of Propane Dehydrogenation on Pt Catalysts*, Oral presentation in the 22nd International Symposium on Chemical Reaction Engineering (ISCRE 22), Maastricht, Netherlands , Sept. 2nd to 5th, 2012.

Financial support:
The Norwegian Research Council (NFR).

Microkinetic modeling of ethylene oxychlorination

Postdoctoral Fellow: Dr. Jun Zhu
Supervisor: Prof. De Chen

Ethylene oxychlorination is an industrial process of great importance. Traditionally, $CuCl_2/Al_2O_3$ with different dopants (KCl, LaCl) is used as a catalyst for the reaction. Although many kinetic models have been proposed, none of them is able to describe the reaction over a wide temperature interval. The goal of this study was to carry out the series of transient catalytic experiments of particular reactions of the catalytic cycle with using the catalyst without any dopants.

Essential improvement in the process performance, however, could be achieved by the introduction of a three step reaction system, where the regeneration of cuprous chloride is conducted separately. The kinetic study of the process can be divided into three subprocesses. 1) CuCl2 reduce by ethylene to CuCl, 2) the Cu(I) reoxidize by O_2 and 3) the HCl regenerate the Cl content. The present work investigated the transient kinetics of these three steps individually by applying an alternative dynamic method with stepwise supply of reactants. The effects of C_2H_4, O_2 and HCl concentrations were observed quantitatively by the continuous supply of the gaseous reactants to the bed of cupric chloride. Transient response of reactants and products concentrations was directly measured by a mass spectrometer with a selected ion-chromatograph mode. The change of the catalyst, i.e. $CuCl_2/Al_2O_3$, was detected by in-situ UV-vis spectroscopy and also correlated with the MS signal.

Langmuir-Hinshelwood kinetic models were delivered and it was found that the first reaction is the first order with respect to the available Cl concentration and the second reaction of the first order with respect to Cu(I) concentration. The third reaction is proved to react much faster. Moreover, the first reaction, i.e. the chlorination reaction, can be simulated with a two active sites model. Combing the kinetic models of three individual steps, the steady state reaction rate can be well predicted on $CuCl_2/Al_2O_3$.

Publications and presentations in 2012:

1. Jun Zhu, De Chen. *Transient Kinetic Investigation of Ethylene Oxychlorination*. Oral presentation in 15th Nordic Symposium on Catalysis, Åland, Finland, June 10th to 12th, 2012

Financial support:
The project is funded by NTNU and the Norwegian research council through the InGAP center.

SINTEF projects

Hydrotreating

Staff: Research scientist Håkon Bergem, Engineer Camilla Otterlei, SINTEF. Professor Edd A. Blekkan, NTNU

The project aims to improve the performance of the client's commercial hydrotreating units. New fuel specifications and changing crude oil qualities call for continuous development of existing and new refinery processes. We are involved in research aiming at developing new and better catalysts but also process optimization and modeling based on insight into the detailed mechanisms of the actual reactions. The processes are studied in bench- and pilot scale reactors.

Client: Statoil R&D

Refinery operations / Octane processes

Staff: Research scientist Hilde Bjørkan, Engineer Marianne Aune and Senior scientist Torbjørn Gjervan

The project aims to improve the performance of the client's commercial catalytic reforming and isomerisation units. This includes catalyst evaluations, process optimization, general trouble-shooting and education of refinery personnel. The heart of the project is a small-scale pilot unit, but additional chemical or physical characterization tools are used as well.

Client: Statoil R&D

KMB project, Biomass to liquid fuels (BTL)

Thermal reforming of biomass gasification gas

Staff: Senior scientist Torbjørn Gjervan and Research scientist Svatopluk Chytil

A model biomass gasification gas has been thermally reformed in a tubular SiC reactor in the temperature range 1200 – 1500 °C. The model gas mixture had a following composition (vol. %): He (2.07), H2 (32.96), CO (28.01), CH_4 (11.99) and CO_2 (24.97). Upon its dilution with Ar, the effect of reaction temperature, added water (0 – 33 vol. %) and residence time on the CO_2, CH_4 conversions

and H_2, CO yields were studied. It is shown that the reactant conversions as well as the product yields increase with the reaction temperature and residence time. Methane conversion is rather unaffected by the amount of water presented in the system, while the CO_2 conversion decreases significantly with the amount of added water. The H_2 yield is always lower than the CO yield and increases with the amount of added water. The CO yield is negatively influenced by the water content, most likely due to the influence of the water-gas-shift reaction. A significant enhancement of the model gas with CO and H_2 approaching the equilibrium prediction is observed at the extreme conditions (high temperature and long residence time). A possible reaction scheme for the thermal reforming is proposed as based on the kinetic simulation of the experimental results.

Carbon formed in the initial stage of the thermal reforming was characterized by SEM and Raman spectroscopy. The SiO_2 needle-like micro-domains are observed on the top of the reactor heating zone, while the central part of the heating zone is covered by carbon that has a disordered, amorphous structure of a low density. It is proposed that the SiO_2 species presumably formed by the chemical reaction between the reactor wall material and the reactants act as a support to anchor C formed.

H_2S removal from biomass gasification gas

A series of Mn_xO_y - Al_2O_3 based sorbents for H_2S sorption removal have been prepared either by spray-drying (SD) of Al/Mn precursor solutions or by multiple wet-impregnations of two different Mn precursors on various alumina supports. The calcined materials were characterized using N_2 sorption X-ray diffraction, UV-Raman spectroscopy and Temperature programmed reduction. A new experimental set-up has been built for the testing of the sorbents performance under conditions relevant for the biomass gasification gas upgrading.

Publications in 2012:

1. S. Chytil, A. Lind, E. Vanhaecke, E.A. Blekkan, *Energy Procedia*, 26 (2012) 98
2. S. Chytil, C. Li, S. Wang, W. Lee, A. Holmen, E.A. Blekkan, N. Burke, J. Patel, *Hydrothermal reforming of biomass gasification gas*, manuscript in preparation

Catalytic hydrotreatment (HT) of bio-oils towards alkanes

Project category: Fundamental project

Staff: SINTEF Materials and Chemistry, Dept. Process Chemistry, Senior scientist Rune Lødeng, Scientist Håkon Bergem, Chief Scientist Michael W. Stöcker, Scientist Lenka Hannevold
Staff: NTNU, Dept. Chem. Eng., Post. Doc. Sara B. Eiras, Professor Edd A. Blekkan

In this project new non-noble metal based catalyst materials for chemical conversion by hydrogentreating (HDO) of bio-oil is developed. Catalysts based on disperged molybdenum carbide, nitride or phosphide, as active phase on different support materials (Al_2O_3, SiO_2, ZrO_2, TiO_2, mesoporous MCM-41, etc.), are synthesized, characterized and tested with regard to kinetic properties (rates and mechanisms). The carbides and nitrides have been synthesized with temperature programmed reaction in mixture of methane/hydrogen (carbon source) and ammonia (nitrogen source), respectively.

Primarily model components such as phenol or guaiacol have been used as feed (as representatives for lignin). The results show that support properties (surface area, porosity, acidity), amount of active phase, synthesis conditions (steering the formation of the active phase), all are importent for the final catalytic properties in the conversion. The catalysts are characterized by x-ray diffraction (phases/structure), N_2-adsorption (physical surface), CO-chemisorption (active surface and structure), IR-pyridine (acidity). The stability of the carbides are studied thermogravimetrically in presence of hydrogen. The carbidese have so far showed promising properties in therms of the activity, relatively slow deactivation, and high selectivity for breaking the C-O bond in phenol (knock off the –OH group to H_2O).

Publications in 2012:

1. Book chapter: "*Catalytic hydrotreatment of bio-oils for high quality fuels production*" by Rune Lødeng, Lenka Hannevold, Håkon Bergem and Michael Stöcker, in "*The Role of Catalysis for the Sustainable Production of Biofuels and Biochemicals*", edited by K. Triantafyllidis, A. Lappas and M. Stöcker, Accepted /Will be published by Elsevier in 2013.

2. Review paper on HDO catalysis and chemistry: " *Potential of carbide, nitride, and phosphide based as future hydrotreatment (HT) catalyst for processing of bio-oils* " by Sara B. Eiras, Rune Lødeng, Lenka Hannevold, Michael Stöcker, Håkon Bergem, Edd A. Blekkan, submitted, “Catalysis”.

3. Sara B. Eiras, Rune Lødeng, Lenka Hannevold, Michael Stöcker, Håkon Bergem, Edd A. Blekkan, *Catalytic hydrodeoxygenation of phenol over carbides, nitrides and phosphides*, Submitted to Catalysis Today (January 2013)

Funding (2011 – 2012): The Norwegian Research Council

Dehydrogenation of propane over chromium oxide based catalysts

Project category: Industry project

Staff: Senior Scientists Rune Lødeng (Dept. Process Chemistry, SINTEF) and Senior Scientist Magne Lysberg (Dept. Process Technology, SINTEF). Prof. Chen De, Prof. Anders Holmen (Dept. Chem. Eng., NTNU).

Propane dehydrogenation has been studied in a fixed-bed quartz reactor under cycling conditions (DH, Regen.) for comparison of a number of industrial samples at representative working conditions. Kinetic data for the main PDH reaction and the carbon formation has earlier been obtained in the tapered element oscillating microbalance reactor and applied for building kinetic models. A number of candidate commercial catalysts have been investigated and benchmarked. Predictive modeling of an industrial plant performance was part of the project work earlier. Development of reactor models is part of ongoing work.

Client: Borealis Polyolefine, Linz - Austria

Fischer-Tropsch catalysts

Staff: Research Scientist Rune Myrstad (SINTEF), Prof. Anders Holmen and Prof. Edd A. Blekkan (NTNU)

The goal of this project is to support the clients' development of catalysts for the Fischer-Tropsch synthesis by testing and characterization of catalysts.

Client: Statoil R&D and The Research Council of Norway through the InGAP program

Co-based supports and catalysts for conversion of natural gas into synthetic diesel

Staff: Research Scientist Rune Myrstad and Senior Scientist John Walmsley: (SINTEF), Prof. Edd A. Blekkan and Magnus Rønning, (NTNU)

The objective for this knowledge-building project is, by using novel synthesis routes, to develop Co-based Fischer-Tropsch catalyst with improved mechanical and chemical attrition resistance in a slurry environment and with high catalyst activity and stability together with high wax selectivity.

Client: Statoil R&D and The Research Council of Norway through the GASSMAKS program

CO_2 to Methanol and DME

Staff: Research Scientist Rune Myrstad (SINTEF)

The goal of this project is to develop catalyst optimized for the hydrogenation of carbon dioxide to methanol/dimethylether under optimal membrane performance process conditions for the selective removal of water.

Client: EU FP7 (The CARENA project)

Microstructured Reactors for Compact Conversion of Natural Gas to Liquid Fuels

Staff: Research Scientist Rune Myrstad (SINTEF), Prof. Hilde Johnsen Venvik (NTNU)

The objectives of this project are is increased knowledge on microstructured reactor technology for production of liquid fuels from natural gas:
- Fundamental knowledge on hybrid catalyst systems for direct synthesis of DME from synthesis gas in microstructured reactors
- Increased knowledge on the Co-catalyst in microstructured reactors and scale-up issues for a Fischer-Tropsch process

Publications and presentations in 2012:

1. H. Bakhtiary-D., F. Dadgar, F. Hayer, X. K. Phan, R. Myrstad, H. J. Venvik, P. Pfeifer, A. Holmen, *Analysis of external and internal mass transfer at low Reynolds numbers in a multiple-slit packed bed microstructured reactor for synthesis of methanol from syngas*, Ind. Eng. Chem. Res. 51 (42), 2012

Client: The Research Council of Norway through the GASSMAKS program

BRISK

The main activity of BRISK (Biofuels Research Infrastructure for Sharing Knowledge) is to promote collaboration and fund and enable research activities across the 26 partner facilities. Thermal biomass conversion enables wood, energy crops, agricultural wastes and other biogenic materials to be processed into liquids, gases and solids for production of electricity, heat, transport fuels and a wide variety of chemicals. Enhancing biomass utilization without compromising its sustainability is a European energy priority, and is linked to targets for curbing greenhouse gas emissions by 20% by 2020, and 50% by 2050. Energy security and integration with other industrial sectors such as agriculture, also play an important role. Development of advanced biomass conversion processes and biorefineries are key elements in achieving greenhouse gas emissions and security of supply goals. The BRISK network encourages and facilitates cooperative research in the project partners' laboratories. The project idea is that the partners open their facilities to visitors from EU and collaborating countries, and the project pays a travel grant for each approved visit.

Under this programme PhD-student Henrik Romar from the Kokkola University Consortium Chydenius, Finland, spent a month in our laboratories working on his Fischer-Tropsch catalysts.

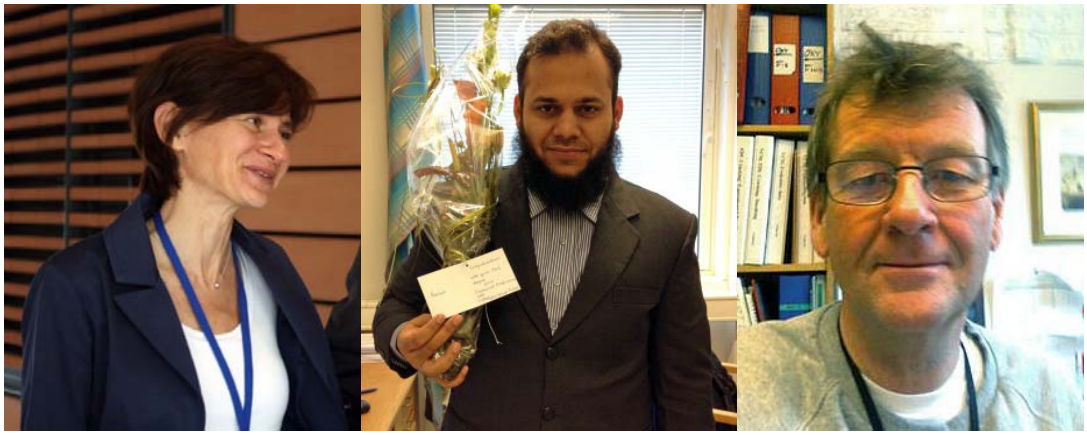
More information: www.briskeu.com
Contact person: Prof. Edd A. Blekkan

Philosophiae Doctor (PhD) theses in 2012

Hassan Jamil Dar*: Gas Phase Oxidative Dehydrogenation of Ethane. Kinetics and Reactor* Doctoral theses at NTNU, 2012:226

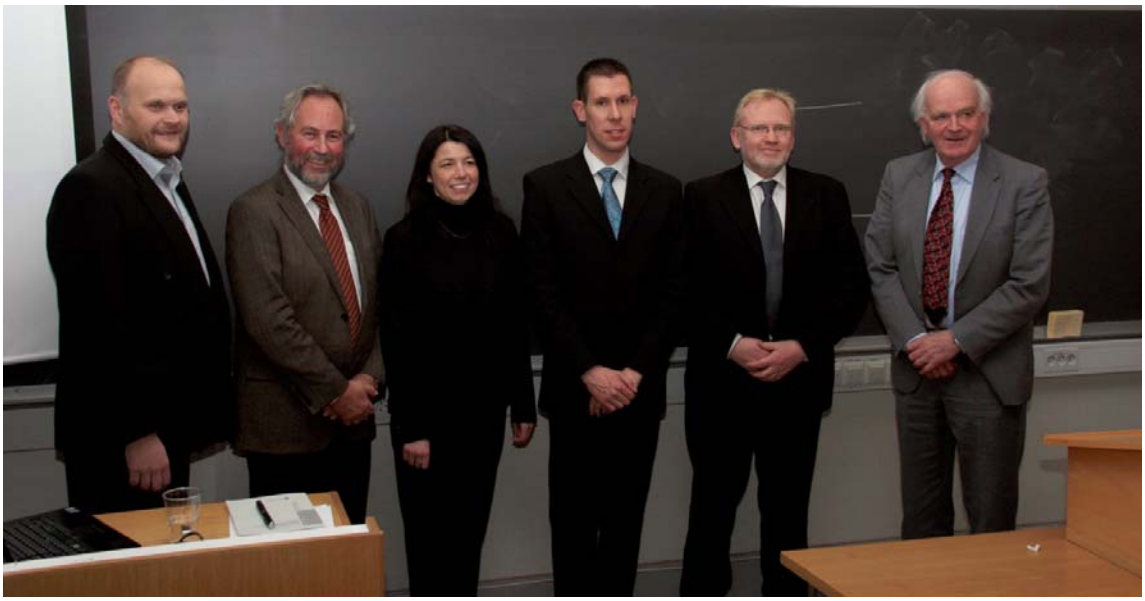
Eleni Patanou: *Adsorption Microcalorimetry Studies on Supported Cobalt Catalysts.* Doctoral theses at NTNU, 2012:247

Paul B. Radstake: *Dehydrogenation of Ethane over Alumina-Supported Pt-Sn Catalysts.* Doctoral theses at NTNU, 2012376



Disputas Hassan Jamil Dar 21/08/2012. From left: Prof. Alessandra Beretta, Dipartimento di Chimica Industriale e Ingegneria Chimica, Politecnico di Milano, Italy (opponent), Dr. Hassan Jamil Dar, Sjefsingeniør Terje Fuglerud, INEOS ChlorVinyls (opponent). Prof. De Chen (supervisor), not shown.

Disputas Eleni Patanou 12/09/2012 .From left: Prof. Edd A. Blekkan (supervisor), Prof. Magnus Rønning (Committee administrator), Prof. Øyvind Weiby Gregersen (Dept. head), Dr. Eleni Patanou, Prof. Aline Auroux, Institut de recherches sur la catalyse et l'environnement de Lyon (IRCELYON - CNRS, France) (opponent), Ass. Prof. Stian Svelle, University of Oslo, Norway (opponent).



Disputas Paul Radstake 14/12/2012. From left: Prof. Magnus Rønning (co-supervisor), Prof. Klaus-Joachim Jens, Høgskolen I Telemark (opponent), Bozena Aeijelts Averink-Silberova (opponent), Dr. Paul Radstake, Prof. Edd A. Blekkan (Committe administrator), Prof. Anders Holmen (supervisor).

Master (Diploma) Students in 2012

Amir Shadman Far*: Alumina supported cobalt catalysts for Fischer-Tropsch synthesis.*

Nina Tung Gynnild: Synthesis of *Fischer –Tropsch catalysts in an autoclave system*

Anette Midttveit: *Ordered mesoporous alumina as support for Fischer-Tropsch catalysts*

Pablo Saz Perez: *Large-scale CNF synthesis*

Gerard Ayuso Virgili: *Kinetic study of oxidative oxychlorination process*

Michael Wycisk: *Co nanoparticles from F-T synthesis*

Juejing Sheng: *Simulation of sorption enhanced steam methane reforming for use in technology assessment of pre-combustion CO2 capture*

Joan Rodriguez-Recasens: *Synthesis and applications of polyaniline nanofibers in*

Christina Carlsen: *Catalytic HDO of bio-oils*

Virginie Marie Therese Herauville: *Catalytic Dehydrogenation of Propane: Oxidative and Non-Oxidative Dehydrogenation of Propane*

Julio Guillermo Martin Montoya: *Adsorption Properties of Supported Cobalt Catalysts Studied via Microcalorimetry*

Sindre Håvik: *Fischer-Tropsch synthesis*

Alexei Pylilo: *Gas-phase pyrolysis and chemical quenching*

Live Nova Næss (Dept. of Physics, co-supervised): *Pd-based Membranes for Hydrogen Separation - Membrane Structure and Hydrogen Sorption and Permeation Behavior*

Group meetings with seminars

Spring 2012

Date	Presenter	Presentation
17.01.12		*Cleaning day issues and HMS/HES*
10.02.12	Magnus Rotan Piotr Ochal	*"Phase composition, microstructure and resistance to attrition of alumina-based supports for Fischer-Tropsch catalysts"* *Carbon-supported Ru@Pt core-shell catalyst for low temperature fuel cells*
17.02.12	Øyvind Gregersen, IKP	*IKP strategy*
02.03.12	Duncan Akporiaye, Kincat/SINTEF	*SINTEF MK Process Chemistry Department – people and research projects*
16.03.12	Rune Myrstad	*Scale-up of microchannel reactors for small scale GTL processes*
30.03.12	Fengliu Lou	*Synthesis of MnO2/aligned carbon nanotubes/Al foil as binder free cathode for high performance lithium ion battery"*
27.04.12	PhD student Francesco Cherubini Department of Energy and Process Engineering, NTNU	*"What is the climate impact of biofuels and bioenergy systems?"*
11.05.12	Hilde Venvik	*Hydrogen fuel cell car test drive/demonstration. Mercedes/Daimler F-cell*
25.05.12	Dr. Bjørn Christian Enger	*On the nature of Fischer-Tropsch synthesis: thermodynamics and catalysis"*
08.06.12	Dr. Knut Grande, Statoil	*Upgrading of Fischer-Tropsch waxes to lubes and transportation fuels*

Fall 2012

Date	Presenter	Presentation
31.08.12		*Introduction of new group members*
14.09.12	Svatopluk Chytil	*Thermal reforming of biomass gasification gas*
12.10.12	Chaoen Li (CSIRO, Melbourne Australia)	*"Gas to Liquid Processes in the Australian Context – CSIRO Research".*
26.10.12	Sara Boullosa Eiras	*Catalytic HDO of Phenol over Supported Mo2C, Mo2N and MoP Catalysts.*
09.11.12	Henrik Romar	*"Finland, Kokkola and Chydenius, a short presentation"*
23.11.12	Odd A. Rokstad	*Acetylene: Chemistry, production and use.*

Courses given by Group Members

TKP4110 Chemical Reaction Engineering

Coordinator: Assoc. Professor Jens –Petter Andreassen

Lecturers: Professor De Chen,
Assoc. Professor Jens-Petter Andreassen,
Professor Heinz Preizig (laboratory exercises)

Semester: Fall
Level: 3th year
Credits: 7.5 SP
Course Plan: Lectures (4 h/week), exercises (6 h/week), self-study (2 h/week)

Objectives:
The course deals with the design of chemical reactors based on the reaction kinetics and the physical conditions in the reactor

Prerequisites:
The course is based on the compulsory courses at the Faculty of Chemistry and Biology, but students from other faculties may take the course as well, possibly after an introductory self-study.

Contents:
The course is divided in a theoretical part and a laboratory part. The theoretical part contains an overview of homogeneous and heterogeneous reaction mechanisms with particular emphasis on the relation between diffusion, heat transfer and reaction rate. Heterogeneous catalysis including reactions between gases, liquids and solid materials is also dealt with. Calculation of conversion and yields in batch reactors and in flow systems i.e. plug flow reactors and continuous-stirred tank reactors. Reactor stability and optimization of the reaction path. The laboratory work includes one exercise related to a topic from the theoretical part.

Teaching form:
The course is given as a combination of lectures, exercises, self-study and laboratory work. Admission to the exam requires that ½ of the exercises are approved. The theoretical part counts for 75% and the laboratory part for 25% of the final mark. Both parts must be passed in order to pass the course.

Course material:
H. Scott Vogler: Elements of Chemical Reaction Engineering. Prentice-Hall, Inc. 4rd ed., 2006.

Exam: Written + exercises

TKP4150 Petrochemistry and oil refining

Responsible: Professor Edd A. Blekkan
Lecturers: Prof. Edd A. Blekkan, Adjunct Prof. Kjell Moljord (Statoil), Prof. Hilde Venvik,

Semester: Spring
Level: 4th year.
Credits: 7.5 SP
Restricted Admission: No

Course Plan: 3 Lectures, 2 hours exercises and 7 hours self-study and projects per week.

Objective:
To provide an overview of the central processes for the conversion and upgrading of oil and natural gas.

Prerequisites:
Basis chemistry and mathematics and course TKP4155 Reaction Kinetics and Catalysis or similar knowledge.

Contents:
Feedstocks, Norwegian oil and gas production, energy from fossil fuels. Oil refining, oil products, refinery design and selected processes, catalytic reforming and isomerization, hydrotreating and hydrocracking, catalytic cracking, treatment of heavy oils, hydrogen balance, environmental concerns, new fuels. Examples of basic, intermediate and end products from petrochemistry. Natural gas and LPG as feedstock, synthesis gas production, preparation and use of hydrogen, methanol synthesis, Fischer–Tropsch, ammonia synthesis. Production of light olefins by steam cracking, dehydrogenation and other routes, use of light olefins.

Teaching:
The course is given as a combination of lectures, exercises, self-study and project work including student presentations.

Course material:
J. Moulijn, M. Makkee and A. van Diepen: Chemical Process Technology Wiley & Sons, 2001, articles and handouts.

Exam: Written

TKP4155 Reaction Kinetics and Catalysis

Responsible: Professor Magnus Rønning
Lecturers: Professor Magnus Rønning and Adj. Professor Erling Rytter.

Semester: Fall
Level: 4th year
Credits: 7.5 SP
Restricted Admission: No
Course Plan: Lectures (4 h/week), exercises (2 h/week), self-study (6 h/week)

Objectives:
Introduction to important principles and methods of heterogeneous and homogeneous catalysis.

Prerequisites:
Course TKP4110 Chemical Reaction Engineering or similar knowledge.

Contents:
The importance of catalysis as a key technology in chemical and petrochemical industry, in energy production and for the protection of the environment. Definition of catalysis, elementary reactions, chain reactions and catalytic sequences. Kinetic modeling. Catalyst preparation and characterization. Adsorption, desorption, surface area and porosity. Modern theories for surfaces and surface reactions. Internal and external mass and heat transfer in catalyst particles. The effect of diffusion on reaction kinetics. Multifunctional catalysis. Catalysis by transition metal complexes. Ziegler-Natta and single-site polymerisation catalysts.

Teaching form:
The course is given as a combination of lectures, exercises and self-study.

Course material:
I. Chorkendorff. J.W. Niemantsverdriet: Concepts of Modern Catalysis and Kinetics, Wiley-VCM.2007. 2nd. Edition

Exam: Written

TKP4190 - Fabrication and Applications of Nanomaterials

Responsible: Associate Professor Jens-Petter Andreassen
Lecturers: Prof. Hilde Venvik, Prof. Wilhelm Robert Glomm

Semester: Spring
Level: 3/4th year.
Credits: 7.5 SP
Restricted Admission: No
Course Plan: 3 Lectures, 2 hours exercises and 7 hours self-study and assignments per week.

Objective:
To provide an overview of how nanoparticles can be made and applied within chemical processes

Prerequisites:
Basis chemistry and mathematics and course TMT4320 Nanomaterials.

Contents:
The thermodynamic driving force and the kinetics of nucleation and growth of nanoparticles is derived, focusing on precipitation from solutions. Different mechanism for nucleation and crystal growth along with calculations of nucleation and growth rates define the basis for design of different particle populations and applications relevant to research and industry.

The unique optical properties of nanoparticles made of noble metals such as gold and silver (localized surface plasmon resonance, LSPR), and how these can be implemented in detection and diagnostic applications via molecular spectroscopy. Use of nanomaterials such as gold nanoparticles, dendrimers, carbon nanotubes and plant viruses for medical applications such as chemotherapy and gene therapy.

Methods for the fabrication of catalysts and catalyst supports based on precipitation, along with other methods with particular relevance for the catalyst nanostructure and functionality, such as sol-gel and colloid based fabrication. Relevant examples where the significance of particle and pore size has been shown are included (Au, Co, Ni- catalysts and carbon nano fibres (CNF)). A short introduction to catalytic model systems and surface science and their experimental and theoretical application within nanocatalysis.

Teaching:
The course is given as a combination of lectures, compulsory exercises, laboratory demonstrations and project work with student presentations.

TKP4190 – Introduction to nanotechnology

Responsible: Professor Helge Weman, Department of Electronics and Telecommunications

Lecturers: Prof. Helge Weman, Prof. Thomas Tybell, Prof. Hilde Venvik, Prof. P. T. Sikorski, Assoc. Prof. R. Nydal

Semester: Fall
Level: 1st year.
Credits: 7.5 SP
Restricted Admission: No
Course Plan: 4 Lectures, 4 hours exercises per week.

Objective:
The subject gives an introduction to central themes within nanotechnology, with emphasis on how this cross-disciplinary technology can increase understanding and promote novel products.

Prerequisites: None

Contents:
The course presents an analysis of areas of relevance to subjects such as bionanotechnology, nanostructured materials, and nanoelectronics. The course will focus on common techniques in order to understand the possibilities of nanotechnology. A section on ethical, energy and environmental issues is also presented.

Teaching:
Lectures, mandatory exercises, laboratory demonstrations and group work. A continuous evaluation based on the exercises and group works will be used, each will be graded in percent.

Catalysis and petrochemistry MSc specialization

Coordinator: Professor Edd Anders Blekkan

Course description:

The specialization involves the following modules:

Course on HMS (Health, Environment and Safety) and Laboratory work	
TKP4510 - Catalysis and Petrochemistry, Specialization Project	15 SP
TKP4515 - Catalysis and Petrochemistry, Specialization Course	7.5 SP
Module 1 (KAT) Heterogeneous catalysis. Advanced course	3.75 SP
Module 2 (KEM) Energy and environmental catalysis	3.75 SP

2 modules must be chosen, other modules are also electable. The modules give an overall description of the field catalysis and petrochemistry. However, the modules may also be combined with modules from other specializations such as polymer chemistry and reactor technology. Catalysis and petrochemistry laboratory work/project is compulsory for this specialization.

Course on HMS (Health, Environment and Safety) and Laboratory work

Responsible: Professor Hilde J. Venvik

Credits: The course is obligatory and a part of the TKP specialization in catalysis.
Prerequisites: None

Course description:
The goal is to develop a course in HMS (health, environment and safety) covering the activities of the catalysis group. The course is for 5th year students and new Ph.D. students, and is to be held for one week in the beginning of the autumn semester. The goal of the course is

- to give the same qualitative information to everybody working in our laboratories, and thereby improve the safety in the laboratories.
- to improve the attitude to and knowledge in HMS in working life by more teaching and higher demands for this also during the studies.
- to improve the students' competence in using the equipment at hand, and thereby improve the efficiency and the quality of the experimental work.
- to introduce the students to the working environment, and to improve the reliance between all the employees.

Teaching methods: Seminars
Course material: Handouts

TKP4515-1 Heterogeneous catalysis, advanced course

Responsible: Professor Edd Anders Blekkan

Credits: 3.75 SP

Prerequisites:
TKP4155 Reaction kinetics and catalysis or similar knowledge.

Module description:
The module covers selected topics in heterogeneous catalysis: Characterization and surface area measurements of porous materials and heterogeneous catalysts, deactivation, activity measurements, kinetics and transient kinetic methods, catalytic materials such as metals, supported metals, oxides, zeolites and solid acids.

Teaching methods:
Seminars, self-study, exercises/project work with presentations.

Course material:
Articles and excerpts from textbooks.

Language:
English

KP4515-2 Environmental and energy catalysis

Responsible: Professor Hilde J. Venvik

Credits: 3.75 SP
Prerequisites:
TKP4155 Reaction kinetics and catalysis or equivalent knowledge

Module description:
Catalysis occupies an important position within areas such as environmental technology and energy production. Within environmental technology catalysis has become crucial not only for removing of unwanted components such as NOX, sulfur etc., but also for the development of selective processes. The course will give the fundamentals for catalytic processes for purification of exhaust gases (NOX, CO, unburned hydrocarbons etc). Within energy production the focus is on biofuel production, catalytic combustion, production of H2 and catalysis/reactor technology related to fuel cells. Catalysis for clean production will also be an important part of the course.

Teaching methods:
Seminars, self-study, exercises/project work with presentations.

Course material:
Articles and excerpts from textbooks.

Language:
English

Ph.D. courses

KP8132 Applied heterogeneous catalysis

Responsible: Professor De Chen
Lecturers: Prof. Hilde J. Venvik and Prof. De Chen

Credits: 7.5 SP
Prerequisites: TKP4155 Reaction kinetics and catalysis.

Course description:
The course is given every second year, next time in the fall term 2013.
The course gives an introduction to modern theories for the most important groups of heterogeneous catalysts: Metals, metal oxides and zeolites. Examples of industrial applications are included. An overview of the principles for design and preparation of heterogeneous catalysis will be given. The course includes a kinetic description of the different processes involved in a catalytic cycle: Adsorption, surface reaction and desorption in addition to mass and heat transfer. An introduction to different experimental methods for studying catalytic reactions will also be given.

Teaching methods:
Seminars.

Course material:
Selected articles and handouts.

KP8133 Characterization of heterogeneous catalysts

Responsible: Professor Magnus Rønning

Credits: 7.5 SP

Course description:
The course is given every second year, next time in fall term 2014.
In heterogeneous catalysis the reactions take place on the surface of solid materials such as metals, metal oxides and zeolites. It is the conditions on the surface that determines the activity, selectivity and lifetime. Methods for characterization of solid surfaces and of adsorbed components are therefore very important for the understanding of catalytic reactions. The course will give an overview of different methods and a detailed introduction to the use of these methods on catalytic systems. The course covers chemical as well as spectroscopic methods with emphasize on in situ methods.

Course material:
Selected scientific papers.

KP8136 - Modelling of Catalytic Reactions

Responsible: Professor De Chen

Credits: 7.5 SP
Prerequisites: TKP4155 Reaction kinetics and catalysis.

Course description:
The course is given every second year, next time in spring 2013.
The course gives an overview on the methods for building microkinetic model, collecting or theoretically estimating rate constant, and microkinetic simulation. Focus will also on the microkinetic analysis of reaction systems at the atomic level. A project work of microkinetic modeling of a selected reaction system will be included in the course.

Learning methods and activities:
Seminars + project

Course materials:
James A. Dumesic, Dale F. Rudd, Luis M. Aparicio, James E. Rekoske, Andres A. Trenino, The microkinetics of heterogeneous catalysis. ACS professional Reference Book, Washington, DC 1993.
Selected papers

KP8137 - Design and Preparation of Catalytic Materials

Responsible: Professor Hilde Johnsen Venvik
Lecturer: Professor Edd Blekkan

Credits: 7.5 SP

Course description:
The course is given every second year, next time spring 2015.
The course gives an overview of principles for design and preparation of catalytic materials. Synthesis methods for support materials as well as catalytically active phases will be described, e.g. (co-)precipitation, impregnation incl. incipient wetness and ion exchange, deposition-precipitation, sol-gel methods, different methods based on pyrolysis and chemical vapour deposition (CVD). The different steps in the preparation, including drying, calcination and reduction, and parameters that influence/control the final catalyst properties are assessed. Important classes of materials such as alumina, silica and zeolites, as well as structured mesoporous materials (MCM-41, SBA-15) are discussed. Carbon nanofiber (CNF) production by catalytic methods is also included, and an introduction to combinatorial methods for parallel synthesis and/or screening of new catalyst systems will be given. Methods for and challenges connected to synthesis scale-up and industrial processing of heterogeneous catalysts are specifically treated.

Learning objective:
The students should be able to make qualified choices and adjustments regarding catalyst preparation methods and synthesis parameters. To some extent they should be able to assess scale-up and industrial production.

Learning methods and activities:
Seminars

Recommended previous knowledge:
Basic knowledge in solid state chemistry and heterogeneous catalysis is required.

Course materials:
Selected handouts and scientific papers

Publications in 2012

1. B. C. Enger and A. Holmen: *Nickel and Fischer-Tropsch Synthesis*. Catal. Rev.: Sci. and Eng. 54 (4) (2012) 437-488

2. B.C. Enger, R. Lødeng, A. Holmen: *On the nature of elementary reactions from methane to hydrogen over transition metals*. Int. J. Hydrogen Energy 37 (2012) 10418-10424.

3. C. Fan, Y. Zhu, Y. Xu, Y Zhou, X. Zhou, D. Chen*, Origin of synergistic effect over Ni-based bimetallic surfaces: A density functional theory study*. Journal of Chemical Physics 2012 ;Volum 137.(1) s. -

4. D.S.G P. Vidana, J. Walmsley, A. Holmen, D. Chen, H. J.Venvik, *Metal dusting corrosion initiation in conversion of natural gas to synthesis gas*. Energy Procedia 2012 ;Volum 26. s. 125-134

5. D. Chen, K. Moljord, A. Holmen*: A methanol to olefins review: Diffusion, coke formation and deactivation on SAPO type catalysts*. Micropotous Mesoporous Materials 164 (2012) 239-250

6. F. Bimbela, D. Chen, J.G. Ruiz, L. Garcia, A. Arauzo, *Ni/Al coprecipitated catalysts modified with magnesium and copper for the catalytic steam reforming of model compounds from biomass pyrolysis liquids*. Applied Catalysis B: Environmental 2012 ;Volum 119. s. 1-12

7. F.Huang, D. Chen, *Towards the upper bound of electrochemical performance of ACNT@polyaniline arrays as supercapacitors*. Energy & Environmental Science 2012 ;Volum 5.(2) s. 5833-5841

8. F.Huang, F. Lou, D.Chen, *Exploring Aligned-Carbon-Nanotubes@Polyaniline Arrays on Household Al as Supercapacitors*. ChemSusChem 2012 ;Volum 5.(5) s. 888-895

9. G. Gao, C. Xu, D. Chen, V.P. Singh*, Spatial and temporal characteristics of actual evapotranspiration over Haihe River basin in China*. Stochastic environmental research and risk assessment (Print) 2012 ;Volum 26.(5) s. 655-669

10. H. D. Bakhtiary, F.Dadgar, F. Hayer, X. K Phan, R. Myrstad, H.J. Venvik, P. Pfeifer, A. Holmen, *Analysis of External and Internal Mass Transfer at Low Reynolds Numbers in a Multiple-Slit Packed Bed Microstructured Reactor for Synthesis of Methanol from Syngas.* Industrial & Engineering Chemistry Research 2012 ;Volum 51.(42) s. 13574-13579

11. H-Y. Cheng, Y-A. Zhu, Z-J. Sui, X. Zhou, D. Chen, *Modelling of fishbone-type carbon nanofibers with cone-helix structures*. Carbon 2012 ;Volum 50.(12) s. 4359-4372

12. H.J. Dar, S.U. Nanot, K.J. Jens, H. A. Jakobsen, E. Tangstad, D. Chen, *Kinetic Analysis and Upper Bound of Ethylene Yield of Gas Phase Oxidative*

Dehydrogenation of Ethane to Ethylene. Industrial & Engineering Chemistry Research 2012 ;Volum 51.(32) s. 10571-10585

13. I.Tronstad, E.A Blekkan, M-H.Ese, *Isothermal Microcalorimetry as a Tool for Studying Oxidation Stability of Insulating Liquids*, IEEE transactions on dielectrics and electrical insulation 2012 ;Volum 19.(5) s. 1528-1536

14. I-H. Svenum, J.A. Herron, M. Mavrikakis, H.J. Venvik, *Adsorbate-induced segregation in a PdAg membrane model system: Pd3Ag(111)*. Catalysis Today 193(2012) 111-119.

15. J. Fermoso, L. He, D. Chen, *Production of high purity hydrogen by sorption enhanced steam reforming of crude glycerol.* International journal of hydrogen energy 2012;Volum 37.(19) s. 14047-14054

16. J. Fermoso, L.He, D. Chen, *Sorption enhanced steam reforming (SESR): a direct route towards efficient hydrogen production from biomass-derived compounds*. Journal of chemical technology and biotechnology (1986) 2012 ;Volum 87.(10) s. 1367-1374

17. J. Fermoso, F. Rubiera, D. Chen, *Sorption enhanced catalytic steam gasification process: a direct route from lignocellulosic biomass to high purity hydrogen*. Energy & Environmental Science 2012 ;Volum 5.(4) s. 6358-6367

18. J. Restivo, J. J. M. Órfão, M. F. R. Pereira, E. Vanhaecke, M. Rønning, T. Iouranova, L. Kiwi-Minsker, S. Armenise and E. Garcia-Bordejé, *Catalytic ozonation of oxalic acid using carbon nanofibres on macrostructured supports*, Water Sci. Tech. 65(10) (2012), 1854-1862

19. J. Yang, D. Chen, A. Holmen: *Understanding the kinetics and Re promotion of carbon nanotube supported cobalt catalysts by SSITKA*. Catal. Today 186 (2012) 99-108.

20. L. He, D. Chen*, Hydrogen Production from Glucose and Sorbitol by Sorption-Enhanced Steam Reforming: Challenges and Promises*. ChemSusChem 2012 ;Volum 5.(3) s. 587-595

21. M. Yang, Y. Zhu, X. Zhou, J. Sui, D. Chen, *First-Principles Calculations of Propane Dehydrogenation over PtSn Catalysts*. Journal of the American Chemical Society 2012 ;Volum 2.(6) s. 1247-1258

22. N. E. Tsakoumis, A. Voronov, M. Rønning, W. van Beek, Ø. Borg, E. Rytter, A. Holmen: *Fischer–Tropsch synthesis: An XAS/XRPD combined in situ study from catalyst activation to deactivation*. J. Catal. 291 (2012) 138-148.

23. O. Mihai, M. Surma, D. Chen, A. Holmen: *Chemical looping methane partial oxidation: The effect of the crystal size and O content of* $LaFeO_3$ J. Catal. 293 (2012) 175-185.

24. R. Dehgan-Niri, J. C. Walmsley, A. Holmen, P. A. Midgley, E. Rytter, A. H. Dam, A. B. Hungria, J. C. Hernandez-Garrido, D. Chen: *Nanoconfinement of Ni clusters*

towards a high sintering resistance of steam methane reforming catalysts. Catal. Sci. Techn., 2 (2012) 2476-2484

25. S. B. Eiras, E. M. M.Vanhaecke, T. Zhao, D. Chen, A. Holmen, *Reply to the comment submitted by LFC de Oliveira, FRL Faulstich, FMZ Zotin on "Raman spectroscopy and X-ray diffraction study of the phase transformation of ZrO2-Al2O3 and CeO2-Al2O3 nanocomposites*" Catalysis Today 2012 ;Volum 187.(1) s. 217-217

26. S. Rane, Ø. Borg, E. Rytter, A. Holmen: *Relation between hydrocarbon selectivities and particle size for alumina supported cobalt Fischer-Tropsch catalysts*. Appl. Catal. A: General, 437-438 (2012) 10-17.

27. S. Chytil, A. Lind, E. Vanhaecke, E. A. Blekkan, Preparation and Characterization of MnxOy-Al2O3 Sorbents for H2S Removal from Biomass Gasification Gas, Energy Procedia 26 (2012) 98.

28. X. Duan G. Qian, J. Zhou, X. Zhou, D. Chen, W. Yuan, *Flat interface mediated synthesis of platelet carbon nanofibers on Fe nanoparticles*. Catalysis Today 2012 ;Volum 186.(1) s. 48-53

29. X.Z. Duan, J. Ji, Q. Jian, F. Gang, Z. Chen, Z. Yian, X. Zhou, D. Chen, W.Yuan, *Ammonia decomposition on Fe(110), Co(111) and Ni(111) surfaces: A density functional theory study.* Journal of Molecular Catalysis A: Chemical 2012 ;Volum 357. s. 81-86

30. X. Duan, G. Qian, C. Fan, Y. Zhu, X. Zhou, D. Chen, W. Yuan, *First-principles calculations of ammonia decomposition on Ni(110) surface*. Surface Science 2012 ;Volum 606.(3-4) s. 549-553

31. X. Duan, G. Qian, X. Zhou, D. Chen, W. Yuan, *MCM-41 supported Co-Mo bimetallic catalysts for enhanced hydrogen production by ammonia decomposition*. Chemical Engineering Journal 2012 ;Volum 207. s. 103-108

32. Y.Xu, C.Fan, Y. Zhu, P. Li, X. Zhou, D. Chen, W. Yuan, *Effect of Ag on the control of Ni-catalyzed carbon formation: A density functional theory study*. Catalysis Today 2012 ;Volum 186.(1) s. 54-62

Presentations in 2012

1. A. H. Lillebø, S. Håvik, E.A. Blekkan, A. Holmen*: SiC as support for Co-based Fischer-Tropsch catalysts*. Poster. 15th Nordic Symposium on Catalysis, June 10-16 2012, Mariehamn, Åland.

2. A. H. Lillebø, E. Rytter, E. Blekkan, E. Patanou, A. Holmen: *Effect of Alkali on Co-based Fischer-Tropsch Catalysts*. Lecture. SynFuel 2012 Symposium, June 29-30 2012, Munich, Germany.

3. A. H. Lillebø, S. Håvik, E. A. Blekkan, A. Holmen, *SiC as support material for Co-based Fischer-Tropsch catalysts*. 15th Nordic Symposium on Catalysis; 2012-06-10 - 2012-06-12

4. B.C. Enger*, A. Holmen: *On the nature of Fischer-Tropsch synthesis: thermodynamics and catalysis*. Lecture. 15th Nordic Symposium on Catalysis, June 10-16 2012, Mariehamn, Åland.

5. B.C. Enger, J. Yang, D. Chen, A. Holmen: *Reaction mechanisms for CO hydrogenation: Alternative rate determining steps based on SSITKA-studies*. Poster. SynFuel 2012 Symposium, June 29-30 2012, Munich, Germany.

6. B.C. Enger, A. Holmen: *The cobalt particle size effect in Fischer-Tropsch synthesis: some perspectives based on statistics and particle size distributions*. Poster. 15th International Congress on Catalysis. July 1-6 2012, Munich, Germany.

7. D. S. G. P. Vidana, J. Walmsley, D. Chen, A. Holmen, H. J.Venvik, *Investigation of metal dusting corrosion initiation in natural gas conversion*. 15th Nordic Symposium on Catalysis; 2012-06-10 - 2012-06-12

8. D. S. G.P. Vidana, J. Walmsley, H. J. Venvik, *Investigation of metal dusting corrosion initiation in natural gas conversion*. SYNFUEL 2012, International Symposium on Alternative Clean Synthetic Fuels; 2012-06-29 - 2012-06-30

9. E.A. Blekkan, Biodrivstoff via gass og Fischer-Tropsch syntese: Katalytiske utfordringer. Teknologisk møteplass - Bioenergi og biodrivstoff(NFR); 2012-06-14

10. E.A. Blekkan, *Biomass to liquid fuels: The gasification route*. Technoport 2012; 2012-04-16 - 2012-04-18

11. E. A. Blekkan, *Fra trevirke til diesel*. Transportforskning 2012; 2012-09-03

12. E. Patanou, E. Z. Tveten, D. Chen, A. Holmen, E. A. Blekkan, *Microcalorimetric studies of H2 and CO suppported catalysts for Fischer-Tropsch synthesis*. Syngas Convention; 2012-04-01 - 2012-04-04

13. E. Patanou, D. Chen, E. A. Blekkan, *Adsorption of H2 and CO on cobalt supported catalysts for the FT synthesis studied by microcalorimetry - effect of cobalt particle size*. 15th International Congress on Catalysis; 2012-07-01 - 2012-07-07

14. F. Lou, H. Zhou, F. Huang, F. Vullum, D. Chen. *Synthesis of MnO2/Aligned Carbon Nanotubes/Aluminium Foil 3D Nanomaterials as Binder Free Cathode for High Performance Lithium Ion Battery*, Oral presentation, International conference of Carbon, Poland

15. F. Lou, H. Zhou, F. Huang, F. Vullum, D. Chen. *Synthesis of MnO2/Aligned Carbon Nanotubes/Aluminium Foil 3D Nanomaterials as Binder Free Cathode for High Performance Lithium Ion Battery*, Invited presentation, The World Resources Forum (WRF) conference 21-23 Oct. 2012, China.

16. Hilde Johnsen Venvik.
    Co surface science revisited. NordForsk network on "*Atomistic design of new catalysts*"; 2012-11-29 - 2012-11-30

17. Hilde Johnsen Venvik.
    Hvordan kan ressursene i nord best utnyttes?. Barentshavkonferansen; 2012-04-23 - 2012-04-25

18. I-H.Svenum, J. A. Herron, M. Mavrikakis, H. J. Venvik, *Co-adsorption of H and CO on a Pd-Ag membrane model system: Pd3Ag(111).* 12th International Conference on Inorganic Membranes; 2012-07-09 - 2012-07-13

19. I-H. Svenum, J. A. Herron, M. Marvikakis, H. J. Venvik, *Co-adsorption of hydrogen and carbon monoxide on Pd3Ag(111)*. 15th Nordic Symposium on Catalysis; 2012-07-10 - 2012-07-12

20. I-H. Svenum, J. A. Herron, M. Marvikakis, Manos; H. J. Venvik,
    Modelling of adsorption on Pd3Ag alloy surfaces. Seminar in connection with the appointment of Professor Jens Nørskov, Stanford University as a Honorary Doctor at NTNU; 2012-05-31

21. I -H. Svenum, J. A. Herron, M. Mavrikakis, H. J. Venvik, *Adsorbate-induced segregation and coadsorption on a Pd-Ag membrane model system*. 14th International Conference on Theoretical Aspects of Catalysis; 2012-06-26 - 2012-06-30

22. I - H.Svenum, J. A. Herron, M. Mavrikakis, H. J. Venvik*, Adsorbate-induced segregation and coadsorption on a Pd-Ag membrane model system*. 14th International Conference on Theoretical Aspects of Catalysis; 2012-06-26 - 2012-06-30

23. J. Fermoso, J. Zhu, D. Chen. Co-Ni catalysts for high party hydrogen production from biomass derived oxygenates. International Conference on Catalysis 2012. Jun 31st – July 6th 2012, Munich, Germany.

24. J. Yang, J. Zhu, A. Lillebø, D. Chen, A. Holmen*: Effect of interfacial properties of hierarchically structured Co catalysts on Fischer-Tropsch synthesis*. Lecture. SynFuel 2012 Symposium, June 29-30 2012, Munich, Germany.

25. J. Yang*, D. Chen, A. Holmen: *New approach for kinetic modelling of Fischer-Tropsch on cobalt based catalysts*. Lecture. 15th International Congress on Catalysis. July 1-6 2012, Munich, Germany.

26. J. Yang, D. Chen, A. Holmen. *Tuning H2 and CO adsorption properties to change product distributions for cobalt catalysts by surface alloy with other metals*, poster presentation, Nordic symposium in catalysis, June 10-12 2012, Finland.

27. J. Zhu, D. Chen, M. Yang, Y. Yu, X. Yu, X. Zhou, A. Holmen: *Selective C-H and C-C Bond Activation of Propane on Platinum Nanoparticles with Different Sizes and Shapes*. Poster. 15th International Congress on Catalysis. July 1-6 2012, Munich, Germany

28. J.Zhu, Virgili, Fuglerud, D. Chen, *Transient kinetic investigation of ethylene oxychlorination*. Oral presentation, Nordic symposium on catalysis, June 10-12, 2012, Finland.

29. M. Ojeda, J.M. Gonzalez-Carballo, J. Yang, A. Holmen, S. Garcia-Roderigues, J-L-G. Fierro: Catalytic effects of rutenium particle size on the Fischer-Tropsch synthesis. Lecture. Syngas Convention, April 1-4 2012, Cape Town, South Africa.

30. M. Rønning*, A. Voronov, N.E. Tsakoumis, G. Voss, W. van Beek, K. Høydalsvik, J.B. Fløystad, D.W. Breiby, J.W. Andreasen, A. Urakawa, A. Holmen: *Surface changes in Fischer-Tropsch catalysts at industrially relevant conditions*. Lecture. 15th Nordic Symposium on Catalysis, June 10-16 2012, Mariehamn, Åland.

31. M. Rønning, A. Voronov, N.E. Tsakoumis, G. Voss, W. van Beek, K. Høydalsvik, J.B. Fløystad, D.W. Breiby, J.W. Andreasen, A. Urakawa, A. Holmen: *Multi-technigue characterisation of surface changes in Fischer-Tropsch catalysts at industrially relevant conditions*. Keynote Lecture. SynFuel 2012 Symposium, June 29-30 2012, Munich, Germany.

32. M. Rønning, A. Voronov, N.E. Tsakoumis, G. Voss, W. van Beek, K. Høydalsvik, J.B. Fløystad, D.W. Breiby, J.W. Andreasen, A. Urakawa, A. Holmen, *Multi-technique characterisation of Fischer-Tropsch catalysts at industrially relevant conditions*, Keynote lecture, ICEC2012, 7th edition of the International Conference on Environmental Catalysis. September 2 - 6 2012, Lyon, France

33. M. Rønning, E. Vanhaecke, N. Hammer, D. Chen, *Pd-Cu catalysts on carbon nanomaterials for the reduction of nitrates in water*, 15th Nordic Symposium on Catalysis, June 10-12. 2012, Mariehamn, Finland

34. N. E. Tsakoumis, A. Voronov, M. Rønning, Ø.Borg, E. Rytter, A. Holmen: *In situ investigations of the initial deactivation in Co-based Fischer-Tropsch synthesis.* Lecture. Syngas Convention, April 1-4 2012, Cape Town, South Africa.

35. N. E. Tsakoumis, A. Voronov, M. Rønning, Ø. Borg, E. Rytter, A. Holmen: *Phase transformations through the induction period of γ-Al_2O_3 supported Co-based Fischer-Tropsch catalysts*. Poster. 15th International Congress on Catalysis. July 1-6 2012, Munich, Germany.

36. N. Muthuswamy, J.L.G. de la Fuente, T. Zhao, M. Tsypkin, M. Rønning, F. Seland, S. Sunde, D. Chen, *Platelet carbon nanofibers supported Pt nanoparticles for Fuel cell*

application. International symposium on carbon for catalysis. Oral presentation, Jun 2012, Italy.

37. S. Hosseini, J. Zhu, D. Chen, E.A Blekkan, I Gorelkin, Herauville, T. D.Tran, J Walmsley, M. Rønning. *Selective hydrogen combustion in mixed hydrocarbons over encapsulated Pt clusters, poster presentation*, Nordic symposium on catalysis, June 10-12 2012, Finland

38. S. B Eiras, R. Lødeng, H. Bergem, M. W. Stöcker, Michael L. Hannevold, E. A. Blekkan. *Catalytic hydrodeoxygenation of bio-oil model components over supported molybdenum carbide, nitride and phosphide catalysts*. UBIOCHEM-III; 2012-11-01 - 2012-11-03

39. T. Zhao, M. Rønning, D. Chen, Y. Sun. *Towards efficient catalytic synthesis of graphene based on a carbon diffusion nucleation model*. International Congress on Catalysis 2012, Jun 31st – July 6th, 2012, Munich, Germany.

40. V. Eijsink og E. A. Blekkan, *Visjoner for Norges bidrag til den globale forskningen på 2. generasjons biodrivstoff*. Bioenergidagene 2012 (NoBIO), Hama, November 5-6, 2012.

KinCat
Catalysis Group – SINTEF – NTNU

Seminar Heterogeneous Catalysis

Tuesday, August 28. 2012

Professor Alessandra Beretta, Department of Energy, Politecnico di Milano

Kinetic study of the catalytic partial oxidation of light hydrocarbons:

1 ***Analysis of alternative lab-scale reactors for the determination of the intrinsic kinetics***
2 **Application of spatially resolved sampling techniques for the characterization of adiabatic short contact time reactors**

The seminar will be given at 10:15-12:00 in Auditorium K5, Chemistry Building V.

KinCat
Catalysis Group – SINTEF – NTNU

Seminar
in connection with the appointment of Professor Jens Nørskov, Stanford University as a Honorary Doctor at NTNU

Thursday May 31 2012
Totalrommet, Main Building, NTNU

1245 Coffe

1300 **Professor Anders Holmen**: *Professor Jens Nørskov, Honorary Doctor at NTNU.*

Professor Jens Nørskov, Stanford University, USA: *Catalysis for sustainable energy solutions.*

1400 **Post.doc. Jia Yang, NTNU**: *New approach for kinetic modeling of Fischer-Tropsch synthesis on cobalt based catalysts.*

1430 **Post.doc. Ingeborg-Helene Svenum, NTNU**: *Modelling of adsorption on Pd3Ag surfaces.*

1500 **Professor De Chen, NTNU:** *Towards better understanding of reaction mechanism of F-T synthesis.*

The seminar is open to the public.

Professor Jens Nørskov appointed as an Honorary Doctor at NTNU. From left: Truls Gjestland SINTEF, Professor Jens Nørskov, Rektor Torbjørn Digernes, Professor Anders Holmen

KinCat
Catalysis Group – SINTEF – NTNU

Seminar I:
Kinetic Modeling of Fischer-Tropsch Synthesis

Time: 13:30-15:30, September 27.2012
Place: KV-323

13:30-14:30 Dr. Chao'en Li, CSIRO, Australia,
Kinetic modeling of Fischer-Tropsch Synthesis

14:30-15:30 Dr. Jia Yang, NTNU
Steady-state and transient kinetic modeling for CO methanation on cobalt catalysts

Seminar II:
Kinetic Modeling of Fischer-Tropsch Synthesis

Time: 10:15-12:00, October 1. 2012
Place: KV-323

10:15-10:45 Dr. Jun Zhu, NTNU,
Compact F-T reactor based on oxide/CNT/carbon felt structured Co catalysts

10:45-10:55 Prof. Per-Olaf Årstrand
Brief introduction of kinetic Monte Carlo

10:55-12:00 Prof. De Chen, NTNU
Microkinetic modeling of GTL process

Alumini
PhD students Catalysis group:

Per Åge Sørum
Hydrogenolysis of esters. Conversion of metylformiat to methanol
Defense of thesis: 1982
Current position: Statoil Mongstad

Edd Anders Blekkan.
Characterization and pyrolysis of heavy oils.
Defense of thesis: November 1985
Current position: Professor NTNU.

Dag Schanke.
Hydrogenation of CO over supported iron catalysts.
Defense of thesis: October 1986
Current position: Chief researcher, Statoil

Kjell Moljord
Diffusion og reaksjon i sure organiske ionebyttere: Væskefase dehydratisering av metanol og t-butanol katalysert av sulfonert poly(styrene-divinylbenzen.
Defense of thesis: 1986
Current position: Statoil, Adjunct professor, NTNU

Edvard Bergene
Surface characterization of Pt and Pt/Rh gauze catalysts.
Defense of thesis: March 1990
Current position: Statoil

Rune Lødeng
Title of thesis: A kinetic model for methane directly to methanol.
Defense of thesis: 1991
Current position: Senior researcher, SINTEF Trondheim

Trude Dypvik
Oligomerization of ethene on zeolite ZSM-5 type catalysts
Defense of thesis: January 1992
Current position: Senior advisor, The Research Council of Norway

Ola Olsvik
Thermal coupling of methane
Defense of thesis: 1993
Current position: Statoil

Anne Hoff
CO hydrogenation over cobalt Fischer-Tropsch catalysts.
Defense of thesis: October 1993
Current position: Statoil

Stein Harald Skaare.
Reaction and heat transfer in wall-cooled fixed bed reactor
Defense of thesis: December 1993
Current position: Aibel, Oslo

Odd Arne Bariås
Transient kinetic investigation of the catalytic dehydrogenation of propane
Defense of thesis: December 1993
Current position: Elkem Solar AS

Geir Remo Fredriksen
Hydrogenation of CO on supported cobalt catalysts studied by in situ FTIR spectroscopy
Defense of thesis: December 1993
Current position: Statoil

Arne Grønvold
Conversion of methanol to lower alkenes over molecular sieve-type catalysts
Defense of thesis: September 1994
Current position: Ineos

Sturla Vada
Isotopic transient kinetic investigations of catalytic reactions.
Defense of thesis: October 1994
Current position: Statoil

Rune Prestvik
Characterization of the metal function of a Pt-Re/Al2O3 reforming catalyst.
Defense of thesis: October 1995
Current position: Statoil

Anne-Mette Hilmen
Reduction and reoxidation of cobalt Fischer-Tropsch catalysts
Defense of thesis: October 1996
Current position: Shell, Norway

Karina Heitnes Hofstad
Catalytic oxidation of methane to synthesis gas
Defense of thesis: 1996
Current position: Statoil

Håkon Bergem
Sulfur tolerant zeolite supported platinum catalysts for aromatics hydrogenation.
Defense of thesis: April 1997
Current position: Senior researcher, SINTEF

Staale Førre Jenssen
Catalytic decomposition of NO over metal exchanged zeolites
Defense of thesis: January 1998
Current position: Statoil

Mimmi Kjetså
Etherification of methanol and iso/n-propanol with C4–C6 olefins on a macroporous acid ion exchange resin catalyst
Defense of thesis: May 1998
Current position: Statoil

De Chen
Methanol conversion to light olefins over SAPO-34: Diffusion, coke depositions and shape selective reactions.
Defense of thesis: 1998
Current position: Professor, NTNU

Hans Petter Rebo
Application of the TEOM reactor for adsorption, diffusion and kinetic studies
Defense of thesis: March 1999
Current position: Statoil

Marit Senum Brownrigg
Deactivation and regeneration of bifunctional zeolites
Defense of thesis: August 1999
Current position: Jotun, Dubai.

Ketil Firing Hanssen
Cobalt Fischer-Tropsch catalysts studied by steady-state and transient kinetic methods
Defense of thesis: 1999
Current position: Senior engineer, Det norske veritas (DNV)

Magnus Rønning
Bimetallic catalysts and platinum surfaces studied by X-ray absorption spectroscopy and scanning tunnelling microscopy.
Defense of thesis: February 2000
Current position: Professor, NTNU

Marcus Fathi
Catalytic partial oxidation of methane to synthesis gas.
Defense of thesis: September 2000
Current position: Statoil

Torbjørn Gjervan
Studies of bimetallic particle formation in reforming catalysts.
Defense of thesis: November 2000
Current position: Research director, SINTEF

Thomas Sperle
Steam reforming of hydrocarbons to synthesis gas.
Defense of thesis: October 2001.
Current position: Chief Technical Officer, Resman

Lucie Bednarova
Study of supported Pt-Sn catalysts for propane dehydrogenation.
Defense of thesis: May 2002
Current position: General Motors, Detroit, USA

Sten Viggo Lundbo
Hydrogenation of carbon monoxide over zirconia and modified zirconia catalysts.
Defense of thesis: June 2002.
Current position: Statoil

Leiv Låte
Oxygen-assisted conversion of propane over metal and metal oxide catalysts
Defense of thesis: 2002
Current position: Head of Division, Force Technology, Trondheim

Petr Steiner
Kinetic and deactivation studies of hydrodesulfurization catalysts
Defense of thesis: December 2002
Current position: Manager, Hart Energy Consulting, Belgium.

Bozena Silberova
Oxidative dehydrogenation of ethane and propane at short contact time.
Defense of thesis: January 2003
Current position: Docent, Hogeschool Rotterdam, Netherlands

Christian Aaserud
Model studies of secondary hydrogenation in Fischer-Tropsch synthesis studied by cobalt catalysts.
Defense of thesis: May 2003.
Current position: Gassco

Kjetil Hauge
Oligomerization of isobutene over solid acid catalysts for production of high octane gasoline
Defense of thesis: September 2004.
Current position: Statoil

Thomas Løften
Catalytic isomerisation of light alkanes
Defense of thesis: December 2004
Current position: Statoil Mongstad

Zhixin Yu
Synthesis of carbon nanofibers and carbon nanotubes.
Defense of thesis: January 2005
Current position: Professor, UiS, Stavanger

Kjersti O. Christensen
Steam reforming of methane on different nickel catalysts.
Defense of thesis: March 2005
Current position: Statoil research centre. Trondheim.

Ingrid Aartun
Microstructured reactors for hydrogen production.
Defense of thesis: June 2005
Current position: Statoil, Mongstad

Sølvi Storsæter
Fischer-Tropsch synthesis over cobalt supported cobalt catalysts.
Defense of thesis: June 2005
Current position: Statoil, Mongstad

Erlend Bjørgum
Methane conversion over mixed metal oxides
Defense of thesis: January 2006
Current position: Statoil, Mongstad

Vidar Frøseth
A steady-state isotopic transient kinetic study of Co catalysts on different supports.
Defense of thesis: May 2006
Current position: Statoil, Mongstad

Florian Huber
Nanocrystalline copper-based mixed oxide catalysts for water-gas shift
Defense of thesis: August 2006
Current position: HTE, Germany.

Øyvind Borg
Role of alumina support in cobalt Fischer-Tropsch synthesis.
Defense of thesis: April 2007
Current position: Statoil research centre, Trondheim.

Espen Standal Wangen
Characterisation and pyrolysis of heavy oils
Defense of thesis: May 2007
Current position: Frilansjournalist, Vagant, vigilant, Trondheim.

Hilde Dyrbeck
Selective catalytic oxidation of hydrogen and oxygen-assisted conversion of propane
Defense of thesis: September 2007
Current position: Statoil research centre, Trondheim

Svatopluk Chytil
Platinum supported on mesoporous silica SBA-15: preparation, characterisation and catalytic properties
Defense of thesis: September 2007
Current position: Scientist, SINTEF

Ingvar Kvande
Carbon nanofiber supported platinum catalysts.
Defense of thesis: December 2007

Current position: Researcher,
Bioforsk Økologisk, Tingvoll

Hilde Meland
Preparation and characterization of Cu- and Pt-based water-gas shift catalysts.
Defense of thesis: May 2008
Current position: Researcher,
SINTEF Trondheim.

Silje Fosse Håkonsen
Oxidative dehydrogenation of ethane at short contact times.
Defense of thesis: June 2008
Current position: Researcher,
SINTEF Oslo

Bjørn Christian Enger
Hydrogen production by catalytic partial oxidation of methane.
Defense of thesis: December 2008
Current position: Postdoc, NTNU

Nina Hammer
Au-TiO_2 catalysts supported on carbon nanostructures for CO removal reactions
Defense of thesis: November 2008
Current position: Yara, Porsgrunn

Astrid Lervik Mejdell
Properties and application of 1-5 μm Pd/Ag23wt.% membranes for hydrogen separation
Defense of thesis: May 2009
Current position: Researcher, Statoil

Li He
Sorption enhanced steam reforming of biomass derived compounds
Defence of thesis: January 2010
Current position: Norner, Porsgrunn

Sara Boullosa Eiras
Comparative study of selected catalysts for methane partial oxidation.
Defense of thesis: October 2010
Current position: Researcher,
SINTEF Trondheim

Hamidreza Bakhtiary
Performance assessment of a packed bed microstructured reactor – heat exchanger for methanol synthesis from syngas.
Defense of thesis: November 2010
Current position: Senior researcher,
Det norske veritas (DNV).

Xuyen Kim Phan
Catalyst formulations for use in microstructured reactors for conversion of synthesis gas to liquids.
Defense of thesis: January 2011
Current position: WellChem AS

Fatemeh Hayer
Direct Synthesis of Dimethyl Ether in Microstructured Reactors
Defense of thesis: March 15 2011.
Current position: Aibel, Stavanger

Shreyas Panduran Rane
Relation between Catalyst Properties and Selectivity in Fischer-Tropsch Synthesis
Defense of thesis: May 2011
Current position: Trondheim
Forskning og Utvikling (TFoU)

Fan Huang
3D Carbon/polyaniline Nanostructures for Energy Storage
Defense of thesis: August 2011
Current position: Jotun, Sandefjord

Oana Mihai
Partial Oxidation of Methane by Chemical Looping
Defense of thesis: September 2011
Current position: Post.doc.
Chalmers, Sweden

Jia Yang
A steady-State Isotopic Transient Kinetic Study of Cobalt Catalysts: Mechanistic Insights and Effect of Cobalt Particle Size, Supports and Promoters.
Defense of thesis: October 2011
Current position: Post.doc. NTNU

Nikolaos E. Tsakoumis
Deactivation of cobalt based Fischer-Tropsch synthesis catalysts
Defense of thesis: November 2011
Current position: Post.doc. NTNU

Kazi Saima Sultana
Calcium Based CO_2 Acceptors for Sorption Enhanced Steam Methane Reforming
Defense of thesis: November 2011

Navaneethan Muthuswany
Platinum based Catalysts for Methanol Fuel Cells: Metal Clusters and Carbon Supports.
Defense of thesis: December 2011
Current positions: Post.doc. NTNU

Hassan Jamil Dar
Gas Phase Oxidative Dehydrogenation of Ethane, Kinetics and Reactor Simulation
Defense of thesis: August 2012

Eleni Patanou
Adsorption Microcalorimetry studies on Cobalt Catalysts
Defense of thesis: September 2012
Current position: Post.doc. NTNU

Paul Radstake
Dehydrogenation of Ethane over Alumina-Supported Pt-Sn Catalysts
Defense of thesis: December 2012