Annual Report

2016

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.

KinCat addresses:

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Annual Report 2016
KINCAT
Strong Point Centre Kinetics and Catalysis

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KinCat Members
Catalysis Group, Department of Chemical Engineering

Academic staff:

Professor Edd A. Blekkan
Professor De Chen
Professor Magnus Rønning
Professor Hilde J. Venvik
Assoc. Professor Jia Yang
Professor Em. Anders Holmen
Professor Em. Erling Rytter
Adjunct Professor Kjell Moljord
Assoc. Prof. (50%) Estelle Marie M. Vanhaecke

SFI-coordinator:

Coordinator (50%) Estelle Marie M. Vanhaecke
Coordinator (50%) Nikolaos Tsakoumis (from 01.04 2017)

Laboratory personnel:

Engineer Karin Wiggen Dragsten
Senior Engineer Cristian Ledesma Rodriguez (until 01.07 2016)
Senior Engineer Estelle Vanhaecke (from 01.07 2016)

Doctoral students 2016/2017:

Martina Francisca Baidoo
Ole H. Bjørkedal
Marthe Emelie Melandsø Buan
Wenyao Chen
Farbod Dadgar
Guifang Fan
Endre Fenes
Ljubisa Gavrilovic
Xiaoyang Guo
Ida Hjort
Stine Lervold
Yahao Li
Shirley Elisabeth Liland
Juntian Niu
Eirik Østbye Pedersen
Samuel Regli
Haakon Rui
Ata Raul ul Salman
Marie Døvre Strømsheim
Yalan Wang
Xuehang Wang
Cornelis Gerardus van der Wijst
Michael Markus Wycisk
Isaac Yeboah

Postdoctoral fellows 2016/2017

Xavier Auvray
Qingjun Chen
Andrea Cognigni
Mari Helene Farstad
Daham Gunawardana
Li He
Victoria Gil Matellanes
Eleni Patanou
Yanying Qi
Nikolaos Tsakoumis
Diego Alexander Pena Zapata

Visitors:
Professor Ivan Bogoev, Institute of Catalysis, Bulgarian Academy of Sciences, Bulgaria
Ting Cui, Tsinghua University, China
Di Wang, East China University of Science and Technology, China.

Technical and administrative staff shared with other groups at the Department of Chemical Engineering:

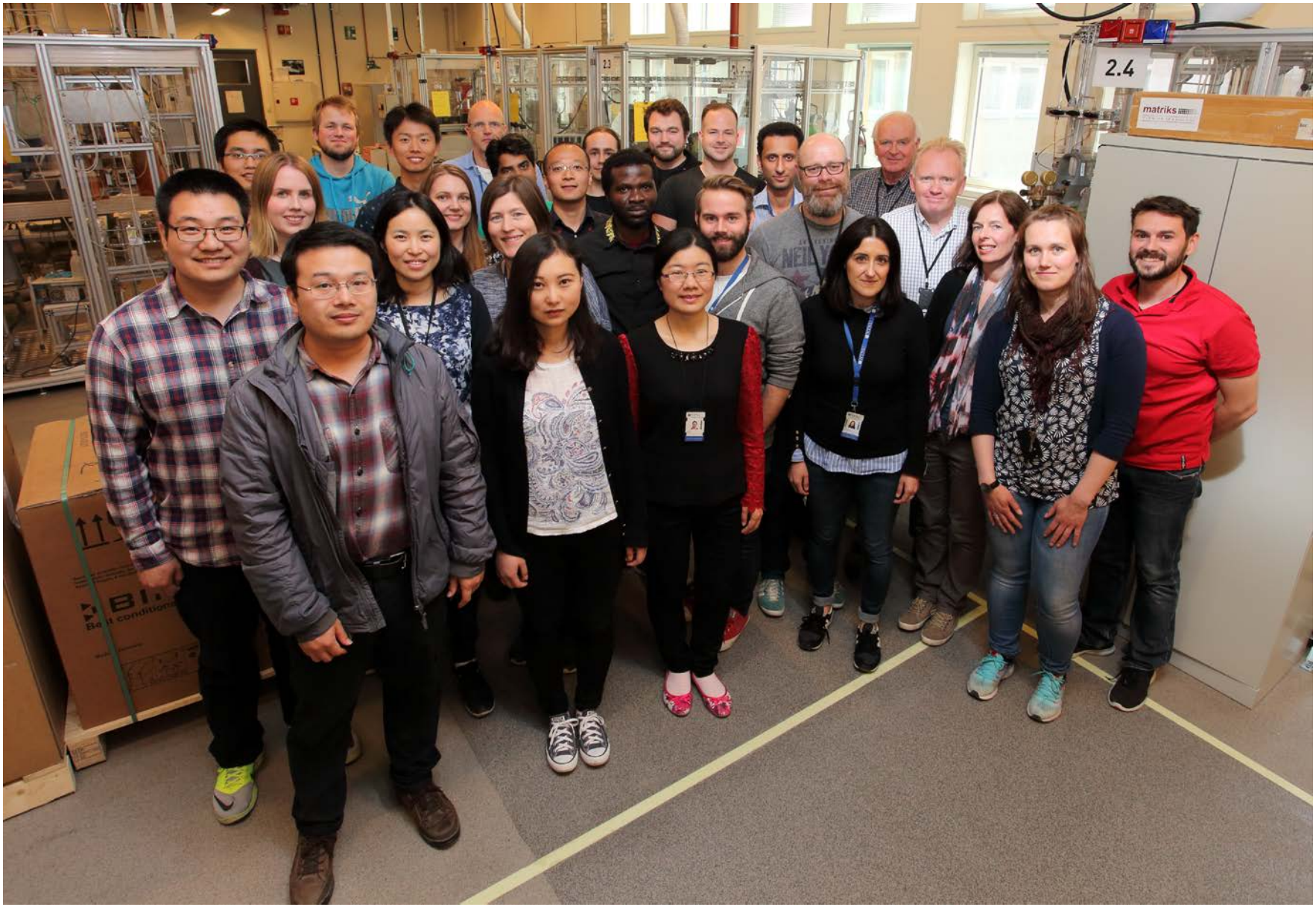
Harry T. Brun
Jan Morten Roel
Mikael Hammer
Erland Strendo

SINTEF Materials and Chemistry, Department of Kinetics and Catalysis

Administration:
Research Manager Torbjørn Gjervan
Senior-/Project Secretary Kirsti Blomsøy

Research scientists:
Research Scientist Håkon Bergem
Research Scientist Svatopluk Chytil
Research Scientist Hilde Bjørkan
Senior Scientist Bjørn Christian Enger
Research Scientist Jia Yang (until 01.11.16)
Senior Scientist Rune Lødeng
Research Scientist Rune Myrstad
Research Scientist Kumar R. Rout

Laboratory personnel
Senior Engineer Camilla Otterlei



Fourth row: Wenyao Chen, Endre Fenes, Xiaoyang Guo, Rune Myrstad, Eirik Østbye Pedersen, Ole H. Bjørkedal, Samuel Regli, Anders Holmen
Third row: Stine Lervold, Shirley Liland, Kumar Rout, Juntian Niu, Ata Salman
Second row: Yahao Li, Jia Yang, Hilde Bjørkan, Isaac Yeboah, Håkon Bergem, Edd Blekkan
First row: Quingjun Chen, Yalan Wang, Guifang Fan, Haakon M. Rui, Victoria Gil, Camilla Otterlei, Karin W. Dragsten, Nikolaos Tsakuomis

Not present: De Chen, Magnus Rønning, Hilde Venvik, Erling Rytter, Kjell Moljord, Estelle Vanhaecke, Marie Strømsheim, Cornelis van der Wijst, Ljubisa Gavrilovic, Mari Helene Farstad, Li He, Yanying Qi, Bjørn Christian Enger, Rune Lødeng,

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)
- Direct methane conversion

❖ Upgrading of Oil Fractions

- Hydrotreating
- Catalytic reforming/isomerization

❖ Biofuels

- Biomass gasification, reforming, water-gas shift, F-T synthesis
- Catalytic upgrading of bio-oils to biofuels
- Catalytic conversion of platform molecules
- Hydrogen from biomass
- Catalytic liquifaction
- Gas conditioning

❖ High Temperature Chemistry

- Free radical chain reactions
- Partial oxidation of methane and NGL compounds

❖ Environmental Catalysis

- Sulfur reduction by hydrotreating
- Oxidation of CO and hydrocarbons
- Wastewater treatment
- CO_2 conversion
- NO_x abatement

❖ Fundamental Studies of Heterogeneous Catalysis

- Surface science and *in situ* methods

- 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 Nanomaterials, Carbon Nanofibers, Nanotubes and Graphene**

❖ **Photocatalysis**

- Water splitting.
- Photoreforming

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
- Twin fixed-bed reactors
- Conventional microbalance reactors
- Oscillating microbalance reactors (TEOM)
- Membrane reactor laboratory
- CSTR reactors
- Transient kinetics (Steady-State Isotopic Transient Kinetic Analysis)
- Multireactor system for CNF synthesis
- Altamira BenchCat Hybrid
- Autoclave reactors
- CVD reactors

❖ Catalyst Preparation Laboratory

- Spray drier
- Ball mills
- Furnaces

❖ Catalyst Characterization

- Surface area (BET), porosity and pore size distribution
- Chemisorption and adsorption calorimetry
- Temperature programmed methods such as TPR, TPO and TPD
- TGA and DSC
- Raman and UV-VIS (*in situ*)
- FT-IR (*in situ*)
- GC-MS and HPLC
- Pyrolysis GC-MS
- Acidity determination by TPD
- XRF – X-ray fluorescence
- Scanning tunneling microscopy (STM)

- 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.
- Synchrotron radiation HR-PES and APPES are frequently used through MAXIV, ASTRID2 and other facilities.

Highlights from the Activities in 2016

- Dr. Jia Yang was appointed as an Associate Professor in the Catalysis group (NTNU) from Nov. 1 2016.

- Dr. Kumar R. Rout was appointed as a Research Scientist in the Catalysis group (SINTEF) from Sept. 19 2016.

- Three candidates completed their PhD degrees in 2016: Yanying Qi, Farbod Dadgar and Xuehang Wang. The titles of the dissertations and pictures of the candidates/committees/supervisors are enclosed.

- 18 Master students completed their thesis in 2016. Their name and titles are enclosed.

- Professor Magnus Rønning is on a one year Sabbatical leave for 2016/ 2017 with Professors Jens Nørskov and Thomas Jaramillo, Stanford University. USA.

- iCSI – industrial Catalysis Science and Innovation – is our Centre for Research-based Innovation awarded by the Research Council of Norway (SFI) with the industrial partners Yara, KA Rasmussen, Dynea, Inovyn, and Haldor Topsøe, and the academic partners are NTNU, UiO and SINTEF. NTNU is the Centre host with Professor Hilde Venvik as the Centre manager. The Kick off Seminar was arranged on Nov 23-24 2016 and the program for the seminar is enclosed. A description of iCSI is also enclosed.

- The group participated in inGAP (Innovative Natural Gas Processes and Products). InGap is a Centre if Research-based Innovation (SFI) with funding from the Research Council and industry (Statoil, Ineos, Haldor Topsøe AS), and with the participation from the University of Oslo, SINTEF, NTNU. The closing date of the inGAP was March 2015, but the last PhD/Post.doc's will finish in 2017.

- The group is a research partner in BIO4FUELS, a Centre for Environment -friendly Energy Research (FME), hosted by The Norwegian University of Life Sciences (NMBU). The Center has a total budget of around 270 MNOK over 8 years, and covers all important value-chains for conversion of lignocellulosic biomass to biofuels. User partners are key national and

international industries, as well as forestry owners and regional authorities. Our activities are related to catalytic processes for the production of biofuels and chemicals from biomass.

- The group was the conference host of the 11th Natural Gas Conversion Symposium (NGCS11) in Tromsø June 5-9 2016. The conference was sponsored by the Research Council of Norway (RCN) GASSMAKS program and by ExxonMobil, Shell and Haldor Topsøe. The local organizing committee had members representing the Norwegian gas conversion community – RCN, NTNU, SINTEF, UiO and INEOS – and the conference chairs were Hilde Venvik and Anders Holmen.

- The group is coordinating one EU-project and participates in several other EU-projects and networks. The group runs several projects within large national research programs such as GASSMAKS and ENERGIX.

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

- The catalysis group runs a bi-weekly seminar. The programs are enclosed.

- Group members participated with invited and keynote lectures at several national and international conferences. The titles of the lectures are enclosed.

- Strategic support from NTNU consisting of PhD fellowships and financial support.

iCSI – industrial Catalysis Science and Innovation for a competitive and sustainable process industry

iCSI is a Centre for research based innovation (SFI) granted 2015-23 by the Research Council of Norway. iCSI includes the industrial partners Yara, K.A. Rasmussen, Dynea, Inovyn and Haldor Topsøe AS and the research partners University of Oslo (UiO), SINTEF and NTNU. The total iCSI budget is MNOK192. The KinCat group at NTNU is the host with Professor Hilde Venvik as the Centre manager and Dr. Estelle Vanhaecke as Centre coordinator. iCSI is organized in 6 Industrial Innovation Areas (IIA) with participation from 3-5 partners in each area.

The iCSI main objective is *to boost industrial innovation and competitiveness* as well as to provide *efficient, low-emission process technology* in its six defined Industrial Innovation Areas through tree basic pillars:

- Improved understanding of the kinetics and chemistry of the catalytic processes of the industrial partners as a basis for performance enhancement and process optimization.
- Synergy between applied and basic research, competence-building and education through interaction between industry, research institutes and universities.
- Development of new materials and methods (experimental and theoretical) that strengthen the industrial value creation and impact the research frontier.

2016 was the ***first full operational year*** of iCSI with all contracts, plans and budgets coming into place. The recruitment of PhD candidates and postdoctoral fellows for the first 4-year period is close to complete and the Centre is proud to present its motivated and competent personnel that together with a large number of NTNU and UiO Master Students chose to work within iCSI.

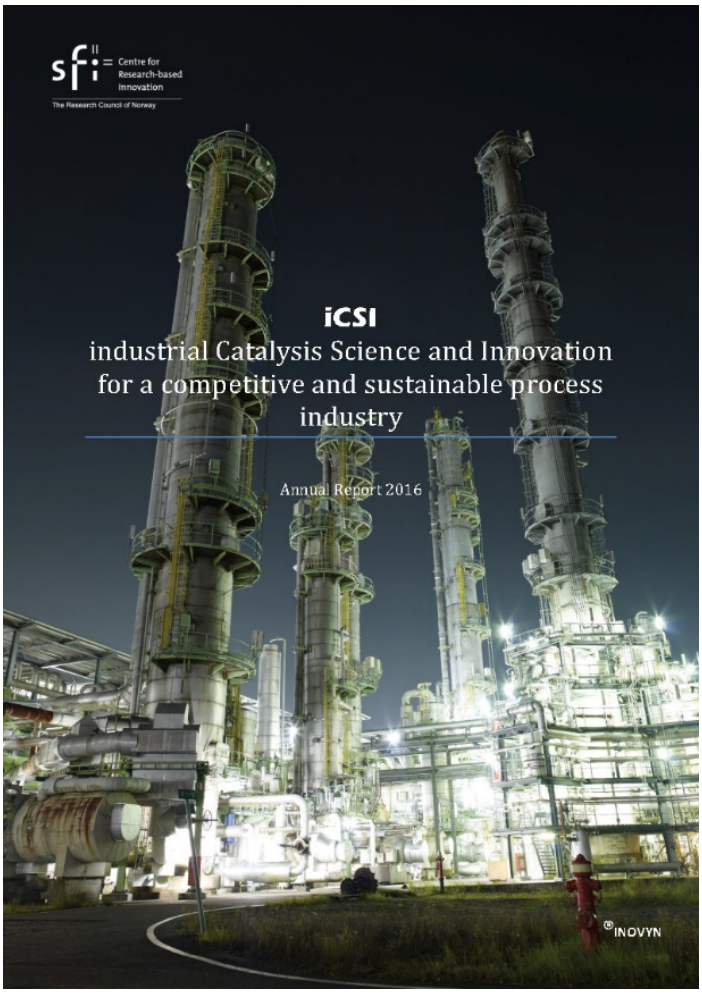
The iCSI Centre is pleased to announce the establishment of its ***Scientific Advisory Committee*** (SAC). Professor Alessandra Beretta (Politecnico di Milano), Professor Enrique Iglesia (UC Berkeley) and Professor Graham Hutchings (Cardiff University) are scientists from prominent institutions who have excelled within iCSI relevant areas of heterogeneous catalysis and represent the international research forefront. They have accepted to advise and be critical, but most importantly to serve as an inspiration to the young iCSI scientists.

The ***iCSI Kick-off meeting*** was held in November 23-24 in Trondheim. 50 participants attended the meeting, with all the industry partners represented and all the PhD and Postdocs present. Prof. Alessandra Beretta (SAC) gave an inspiring and highly relevant lecture on her efforts to combine kinetic analysis and characterization in investigating catalytic partial oxidation of hydrocarbons. Both the scientific and the social program was a success, providing inspiration and ideas across the IIAs and work packages, potential new collaborations within the Centre, as well as new friends.

The ***first iCSI paper*** in a peer-reviewed journal has been published. "*Highly Active and Stable CeO_2-Promoted $CuCl_2/Al_2O_3$ Oxychlorination Catalysts Developed by Rational Design Using a Rate Diagram of the Catalytic Cycle*", by K. R. Rout, E. Fenes, M. F. Baidoo, R. Abdollahi, T. Fuglerud, D. Chen, appeared in *ACS Catalysis* thanks to the collaboration between NTNU, SINTEF and the industry partner INOVYN within the Industrial Innovation Area 4. Objectives, results and dissemination from individual work packages are found in the iCSI Annual report, as well as in the following pages of the KinCat annual report for KinCat associated activities.

In addition, iCSI researchers have given ***41 presentations*** at national and international conferences. Among these are plenary, invited and keynote lectures at NGCS11 (Tromsø), 6th EuChemS Chemistry Congress (Sevilla), and 11th International Congress of Catalysis (Beijing) by Prof. Unni Olsbye (UiO) and Prof. De Chen (NTNU). Some of our PhDs and post docs have attended international courses within state-of-the-art catalysis research, and iCSI researchers lectured at the "Molecules@Surfaces" International Winter School in Bardonnecchia (Italy).

Read more at the iCSI web site where you may also find the iCSI Annual Report 2016:
https://www.ntnu.edu/icsi



Ph.D. Candidates and Postdoctoral Projects

Catalysts for NOx-reduction in maritime transportation

Ph.D. Candidate: Ole Håvik Bjørkedal
Supervisor: Magnus Rønning
Co-supervisor: Rune Lødeng

Coming regulations for maritime nitrogen oxide (NOx) emissions are expected to create a demand for non-toxic NOx-reduction catalysts able to perform at a wide range of operating conditions with special regards to oxygen content and temperature in the exhaust stream. Liquefied Natural Gas (LNG) is becoming more attractive as maritime fuel, due to its increasing supply and opportunity for more efficient and cleaner combustion. However, the combustion process is usually performed with surplus oxygen to minimize the risk of methane slip. Such conditions facilitate generation of thermal NOx, which must be reduced downstream of the engine.

The goal of the project is to develop catalysts for Selective Catalytic Reduction (SCR) under relevant conditions for LNG-propelled ships, as well as reaching a better understanding of the role of the support in SCR-catalysis.

Some zeolites (e.g. ZSM-5) have been investigated as supports for SCR-catalysis with promising results, possibly due to their high specific surface area and surface acidic sites. In this project, ordered mesoporous alumina will be investigated as support material. A sol-gel synthesis with a structure directing surfactant allows for tuning the pore size of the alumina as well as a narrow pore size distribution. In addition, a solid acid will be introduced in an attempt to tune the nature and abundance of surface acidic sites on the support. An active metal component (initially Fe and Cu) will be deposited on the support. A small scale reactor system is being purchased, and will be used to investigate the effects of porosity and acidity, as well as the overall performance of the catalysts.

Funding:
The project is funded by the Norwegian Research Council through the EmX 2025 program.

Nitrogen-doped Carbon Nanofibers for the Oxygen Reduction Reaction

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

Nitrogen-doped carbon nanomaterials exhibit activity towards the oxygen reduction reaction (ORR), the cathode reaction in fuel cells. These materials could thus be a cheap alternative to replace the high cost noble metal catalysts currently used. However, in acidic conditions the ORR activity and stability of the N-doped carbon catalysts have not been comparable to the traditional Pt/C catalyst. In addition, the nature of the active sites and the role of the transition metal used as carbon growth catalyst still remain unclear. Efforts should therefore be made to understand the active site structure in N-doped carbon nanomaterials so that the ORR activity can be further improved. In the present work, a systematic evaluation of

the ORR on nitrogen-doped carbon nanofibers (N-CNFs) is performed and the possible active sites explored.

A catalytic chemical vapor deposition method is employed to grown N-CNFs from Fe and Ni particles on the surface of expanded graphite using NH_3 as nitrogen precursor and CO or C_2H_4 as carbon precursors. The properties of the N-CNFs are tailored by varying the synthesis conditions such as synthesis temperature and NH_3-partial pressure. The electrocatalytic activity for the oxygen reduction is tested by performing linear sweep voltammetry in O_2-saturated acidic and alkaline electrolytes. A rotating ring disk electrode with a Pt-ring is employed to measure the selectivity towards the four electron oxygen reduction. Careful analysis using XPS, BET, TPO, XRD and SEM/TEM is performed to correlate the physicochemical properties of the N-CNFs with the catalytic activity. The nature of the active sites for the oxygen reduction is further explored by combining post-treatment of the N-CNFs with TEM/EELS and XAS characterization.

Publications in 2016:

1. M.E.M. Buan, N. Muthuswamy, J.C. Walmsley, D. Chen, M. Rønning, *Nitrogen-doped Carbon Nanofibers on Expanded Graphite as Oxygen Reduction Electrocatalysts*, Carbon, 101 (2016) 191–202.
2. F.Lou, M.E.M. Buan, N. Muthuswamy, J.C. Walmsley, M. Rønning, De Chen, *One-step electrochemical synthesis of tunable nitrogen-doped graphene*, Journal of Materials Chemistry A, 4 (2016), 1233-1243.
3. D. Bokach, S. ten Hoopen, N. Muthuswamy, M. E. M. Buan, M. Rønning, *Nitrogen-doped carbon nanofiber catalyst for ORR in PEM fuel cell stack: performance, durability and market application aspects*, International Journal of Hydrogen Energy, 41 (2016), 17616-17630.

Presentations in 2016:

1. M. E. M. Buan, N. Muthuswamy, J. C. Walmsley, D. Chen, M. Rønning, *Systematic approach to study the origin of the oxygen reduction reaction on N-CNFs*, Oral presentation, 7th International Symposium on Carbon for Catalysis, Strasbourg, France, 13th June 2016.
2. M. E. M. Buan, N. Muthuswamy, A. Cognigni, J. C. Walmsley, D. Chen, M. Rønning, *Nitrogen-doped carbon nanofibers for the oxygen reduction: The role of iron as growth catalyst*, Oral presentation, PRIME 2016, Hawaii, USA, 5th October 2016.

Financial support:

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

Fundamental studies on the roles of potassium in H_2 and CO dissociation in cobalt-based Fischer−Tropsch synthesis

Postdoctoral Fellow : Dr. Qingjun Chen
Supervisor: Prof. Edd A. Blekkan

The Fischer−Tropsch synthesis (FTS) provides an alternative route for the production of clean fuels and key building blocks in the chemical industry using coal-, natural gas-, or biomass-derived syngas as the feedstock. This process receives increasing attention due to possible shortage of oil, low price of alternative feedstocks or environmental concerns. Comparing with iron-based FTS catalysts, cobalt-based catalysts have higher activity per gram catalyst, better stability and lower CO_2 selectivity, and are widely used in natural gas-based FTS. However, it has been demonstrated that trace amounts of alkaline or alkaline earth metals (100~1000 ppm) could result in significant decrease of the FTS activity of cobalt catalyst while it has almost no effect on the cobalt dispersion (measured as the H_2/CO chemisorption amount) and heat of adsorption of H_2 or CO. In this project, density functional theory (DFT) calculations are employed to investigate the role of potassium in cobalt-based FTS.

H_2 and CO activation are key steps in the initiation of the FTS, and thus a fundamental understanding of H_2 and CO activation mechanism on cobalt is of paramount importance. H_2 adsorption and dissociation over hcp cobalt were first calculated on typical clean and K pre-adsorbed facets of hcp cobalt. The results show that K has negligible effect on H adsorption on each exposed surface of hcp cobalt. The dissociation energy barrier of H_2 was very low (0.13eV) on the clean terrace facet (0001). The pre-sorption of K increased the dissociation energy barrier of H_2 to 0.39 eV and slightly inhibited the H_2 dissociation on (0001) facet. On a stepped facet (10-12), we find that the H_2 dissociation energy barrier (0.33 eV) was higher than that on the terrace facet. K inhibited the H_2 dissociation on (10-12) facet with the dissociation barrier of 0.43 eV. On (10-11), (10-15), and a typical corrugated facet (11-20), K also slightly hinders the dissociation of H_2. K species (K and KOH) have similar effect on the H_2 dissociation.

CO adsorption and dissociation was calculated on typical terrace and stepped facets (0001) and (10-12), which are also preferred for K adsorption. CO adsorption calculations indicated that K improved the CO adsorption both on (0001) and (10-12) facets. CO dissociation calculations showed that the energy barrier (2.41 eV) of CO direct dissociation ($CO \rightarrow C+O$) is much higher than that of H-assisted CO dissociations (min.1.41 eV) on the (0001) facet. On the B_5 site of the stepped facet (10-12), the direct dissociation of CO was preferential with the energy barrier of 1.14 eV, which was much lower than the energy barrier over (0001). Pre-adsorbed K (or KOH) caused a slight increase of H-assisted CO dissociation barriers on (0001) but had almost no effect on the CO dissociation barriers on (10-12). It is suggested that the blocking of the most active B_5 site on the stepped facet (10-12) by K is the main reason for the activity decline of the cobalt catalysts. Furthermore it is noted that the decrease of H coverage caused by pre-adsorbed K also results in the decrease of activity and CH_4 selectivity of cobalt catalysts.

Publications and Presentations in 2016:

1. Qingjun Chen, Ingeborg-Helene Svenum, Yanying Qi, Ljubisa Gavrilovic, De Chen, Anders Holmen, Edd A. Blekkan, *Potassium adsorption behaviors on hcp cobalt: A*

density functional theory calculation, the11th Natural Gas Conversion Symposium, *Poster Presentation*, Tromsø, Norway, 5-9 June, 2016.

2. Qingjun Chen, Ingeborg-Helene Svenum, Yanying Qi, Ljubisa Gavrilovic, De Chen, Anders Holmen, Edd A. Blekkan, *Potassium adsorption behavior and its influence on the CO adsorption and activation on hcp cobalt in Fischer-Tropsch synthesis*, the 16th International Congress on Catalysis, *Poster Presentation*, Beijing, China, 3-8 July, 2016.
3. Qingjun Chen, Ingeborg-Helene Svenum, Yanying Qi, Ljubisa Gavrilovic, De Chen, Anders Holmen, Edd A. Blekkan, *Potassium adsorption behavior on hcp cobalt as model systems for the Fischer-Tropsch synthesis: A density functional theory study*, Physical Chemistry Chemical Physics, submitted, 2016.

Financial Support:
This project is financed by the ENERGIX programme in the Norwegian Research Council (project 228741) and computational resources were provided by UNINETT Sigma 2, account no. NN 9355k and NN 9336k.

Development of X-ray modulation-enhanced techniques to study surface reactions at industrially relevant conditions

Postdoctoral Fellow: Andrea Cognigni
Supervisor: Prof. Magnus Rønning

During the last two decades many synchrotron beamlines specialized in X-ray absorption spectroscopy (XAS) have increased their instrumental performance enormously. While recording a single spectrum used to take several tens of minutes, now it can be recorded in less than 10 seconds or even in the order of milliseconds. This has opened up the way to perform *in situ* and *operando* XAS experiments studying transient structures. In such experiments, XAS data are collected as a function of time while changing a variable of the experimental condition such as temperature, concentration, or pressure. It has become routine to collect hundreds of spectra on a single sample. These large datasets have to be treated and the conventional scan by scan data analysis methods have become a time consuming bottleneck. Automated data processing procedures like least square fitting of data with a linear combination (LC) of reference spectra and Principle Component Analysis (PCA) are powerful tools yet have limitations. More precisely LC requires standards and PCA often provides mixed components that are hard to interpret. Several convenient automated data processing procedures like least square fitting of reference spectra exist but are based on assumptions. In this project, we have explored application of multivariate curve resolution with alternating least-squares (MCR-ALS) as a blind-source separation method to efficiently process large data sets from *in situ* X-ray absorption spectroscopy experiments where the sample undergoes a periodic concentration perturbation.

This project has accelerated the capabilities of the beamline to perform modulation-enhanced experiments, i.e. a periodic perturbation of the experimental conditions collected in order to average a number of cycles. This significantly enhances the signal-to-noise ratio of the acquired spectra. A fast, 2D CMOS XRD detector has been installed in order to bring the powder XRD measurement acquisition time in line with the already state of the art Quick EXAFS setup. Both detection systems are now capable of routinely performing modulation-enhanced experiments

The project is a collaboration with the Swiss-Norwegian Beamlines (SNBL), France and the Institute of Chemical Research of Catalonia (ICIQ), Spain.

Presentations

M. Rønning, *Fischer-Tropsch synthesis catalysts: Strategies to enhance the sensitivity of in situ characterization techniques,* Invited lecture: 251st ACS National Meeting, March 13.-17. 2016, San Diego, USA

Funding:
The project is funded by the Research Council of Norway (NFR) through the SYNKNØYT programme.

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

Ph.D. Candidate: Farbod Dadgar
Supervisors: Prof. Hilde J. Venvik, Prof. Anders Holmen, Research Scientist Rune Myrstad

Micro process technology has a great potential for process intensification through equipment size reduction, process simplification and process integration. Such technology can enable the on-site conversion of remote natural or biomass-derived gas to easily transportable hydrocarbons (e.g. methanol, dimethyl ether or Fischer-Tropsch liquids). Dimethyl ether (DME) is increasingly applied as a LPG substitute and as an alternative diesel fuel with high cetane number, negligible CO and particulate matter emissions, and low NO_x. DME is conventionally produced via a two-step process; methanol synthesis from synthesis gas ($CO+H_2$) over a Cu-ZnO-based catalyst followed by methanol dehydration over an acidic catalyst (e.g. γ-alumina, zeolites). A more recent alternative is the thermodynamically and economically more favorable direct synthesis of DME from synthesis gas in a single unit, applying a dual catalyst system containing both methanol synthesis and methanol dehydration functions.

In this project, direct dimethyl ether (DME) synthesis from synthesis gas is studied with regards to the effect that combining methanol synthesis and dehydration in a single reactor can have on the catalytic performance. An integrated microstructured reactor-heat exchanger is being used, for which the high surface-to volume ratio and micro-range flow dimensions enhance the heat and mass transfer. The results obtained confirm the advantage of direct DME synthesis over the two-step process at conditions where syngas conversion to methanol is thermodynamically limited. However, our results show that combining methanol synthesis and dehydration can have a negative effect on the methanol formation kinetics, observable at conditions where the effect of the reverse reaction on methanol synthesis is negligible. The experiments establish that this is linked to the reaction environment created by the dehydration reaction, i.e. higher concentrations of H_2O/CO_2. On the other hand, the studies indicate that – as long as the two catalyst functions are only physically mixed – the prevailing deactivation mechanisms are those of the two reaction system alone, but with some impact of the combined reaction mixture and the conditions. At this relatively low temperature (250°C), accumulation of organic material retained on the catalyst (retardate) leads to deactivation of H-ZSM-5. Moreover, indications are found that the partial pressures of hydrogen and carbon monoxide also affect this deactivation. Partial deactivation of the zeolite's strong acidic sites by sodium improves catalyst stability.

Publications in 2016:

1. Farbod Dadgar, Rune Myrstad, Peter Pfeifer, Anders Holmen, Hilde J. Venvik. *Direct dimethyl ether synthesis from synthesis gas: The influence of methanol dehydration on methanol synthesis reaction.* Catalysis Today 270 (2016) 76-84.
2. Farbod Dadgar, Rune Myrstad, Peter PfeiferAnders HolmenHilde J. Venvik. *Catalyst Deactivation During One-Step Dimethyl Ether Synthesis from Synthesis Gas.* Catal Lett (2017). doi:10.1007/s10562-017-1971-2

Financial support:
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).

Advanced characterization of catalytic model systems

Postdoctoral Fellow: Dr. Mari Helene Farstad
Supervisor: Prof. Hilde J. Venvik

In order to fully understand a particular catalyst function, it is beneficial to investigate the surface of the active catalyst. Unfortunately, the most detailed surface characterization techniques depend on ultra high vacuum (UHV) and relatively well ordered surfaces in order to obtain high precision results. The extrapolation from UHV and models systems to materials and conditions relevant for catalytic processes is not always valid.

During the resent years the possibilities for in-situ investigations has improved considerably, but resolution is still not as good as in UHV and an intimate familiarity with the sample is often necessary in order to successfully interpreted the results. Combining the in-situ measurements with UHV investigations and first principles calculations, as well as other relevant measurements, is therefore of high importance.

In this project, surface science techniques such as scanning tunneling microscopy (STM) and photoemission spectroscopy (PES) is used to investigate metals relevant to industrial catalysis and emissions abatement; Pd-based alloys for hydrogen membrane separation and catalytic oxidation, Co based Fischer-Tropsch catalysts, and methanol oxidation over Ag. The goal is to establish in-situ experimentation methodology for these systems, in particular near ambient pressure photoelectron spectroscopy (NAPPES) utilizing synchrotron light.

In 2016 the STM lab has been upgraded with new electronics for the STM, new ionpump and new turbopump. Experiments in the home lab has been combined with high resolution PES at the Astrid2 synchrotron in Aarhus, Denmark.

Publications and Presentations in 2016:

1. Marie D. Strømsheim, Jan Knudsen, Mari H.Farstad, Linn Sørvik, Xiaoyang Guo, Hilde J. Venvik, and Anne Borg. *Near ambient pressure XPS investigation of CO oxidation over Pd3Au(100)* Accepted, Topics in Catalysis
2. Marie D. Strømsheim, Ingeborg-Helene Svenum, Mari H. Farstad, Zheshen Li, Ljubisa Gavrilovic, Xiaoyang Guo, Stine Lervold, Anne Borg, and Hilde J. Venvik. *Effects of K adsorption on the CO-induced restructuring of Co(11-20).* Accepted, Catalysis Today

3. Fernandes, Vasco Rafael P; Van der Bossche, Maxime; Knudsen, Jan; Farstad, Mari Helene; Gustafson, Johan; Venvik, Hilde Johnsen; Grönbeck, Henrik; Borg, Anne. *Reversed Hysteresis during CO Oxidation over Pd75Ag25(100)*. ACS Catalysis 6 (2016) 4154
4. Farstad, Mari Helene; Strømsheim, Marie Døvre; Svenum, Ingeborg-Helene; Borg, Anne; Venvik, Hilde Johnsen. *The effect of K impurities on Co(11-20) with respect to Fisher-Tropsh catalysis*. CMD26 Oral presentation
5. Farstad, Mari Helene; Ragazzon, Davide; Strømsheim, Marie Døvre; Gustafson, Johan; Sandell, Anders; Borg, Anne. *Oxidation and Reduction of TiOx on Pd(100) and Pd(111).* 17th Nordic Symposium on Catalysis 2016 and iCSI seminar. Poster
6. Farstad, Mari Helene; Strømsheim, Marie Døvre; Knudsen, Jan; Guo, Xiaoyang; Gavrilovic, Ljubisa; Fernandes, Vasco Rafael P; Borg, Anne; Venvik, Hilde Johnsen. *CO oxidation over Pd-based alloys*. CMD26. Poster

Financial support:
The project is funded by the Faculty of Natural Sciences and the Department of Chemical Engineering, NTNU.

Promoter Effects on Ethylene oxychlorination reaction for $CuCl_2/\gamma\text{-}Al_2O_3$ based catalysts

Ph.D. Candidate: Endre Fenes
Supervisor: Prof. De Chen
Co-supervisor: Terje Fuglerud

The ethylene oxychlorination process produces ethylene dichloride (EDC). EDC is a precursor in the production of poly-vinyl chloride; one of the most commonly used polymers throughout the world. The process is catalyzed by $CuCl_2/\gamma\text{-}Al_2O_3$ based catalysts, and consists of three distinct reaction steps in which copper cycles between Cu^{2+} and Cu^{1+} oxidation states: catalyst reduction by ethylene, consuming chlorine from the catalyst, catalyst oxidation and at last, catalyst hydrochlorination.

In this project, the effect of promotors, i.e., mostly alkali, alkali earth and lanthanide elements on turnover frequency, catalytic activity and stability is investigated by applying an operando study, combining mass- and UV-Vis-NIR spectrometry during both transient and steady state experiments. With respect to the non-promoted catalyst, La promotion increased the reduction and oxidation rates, resulting in an increased activity at moderate catalyst stability, while alkali promotion decreased the reduction rate and significantly increased the oxidation rate, resulting in moderate activity at high stability.

Presentations/publications in 2016:

- Rout, K. R. Fenes, E. Baidoo, M. F. Abdollahi, R. Fuglerud, T. Chen, D. Highly active and stable Highly Active and Stable CeO_2-Promoted $CuCl_2/Al_2O_3$ Oxychlorination Catalysts Developed by Rational Design Using a Rate Diagram of the Catalytic Cycle, ACS Catalysis 2016, **6**(10): 7030-7039

- E. Fenes, K. Rout, M.F. Baidoo, T. Fuglerud, D. Chen, Quantitatively defining promotor influence on catalytic activity and stability in ethylene oxychlorination, 11th Natural Gas Conversion Symposium, 2016, Tromsø
- E.Fenes1, M.F. Baidoo1, K.R. Rout2, T. Fuglerud3, D. Chen, Rational Design of Oxychlorination Catalysts based on Kinetic Rate Diagram, iCSI Seminar, Trondheim 2016.
- K. R. Rout, M. F. Baidoo, E. Fenes, J. Zhu, T. Fuglerud, and D. Chen, Understanding of Potassium Promoter Effects on Oxychlorination of Ethylene by Operando Spatial-time Resolved UV-Vis-NIR Spectrometry, Journal of Catalysis, Accepted

Financial support:
The project is a research activity under iCSI – industrial Catalysis Science and Innovation for a competitive and sustainable process industry", which is a National Centre for Research-based Innovation (SFI) granted by the Research Council of Norway.

Influence of alkali species on cobalt-based Fischer-Tropsch catalyst

Ph.D. Candidate: Ljubiša Gavrilović
Supervisor: Prof. Edd A. Blekkan
Co-supervisor: Prof. Hilde J. Venvik

All carbon-containing feedstocks can be converted to liquid fuels via the Fischer-Tropsch (FT) synthesis. Due to the chemistry of the Fischer-Tropsch synthesis is the production of diesel fuel and aviation fuel (jet fuel) particularly attractive. FT diesel has better properties than the crude oil based fuels with respect to the cetane number and absence of aromatic and sulphur compounds, and the jet fuel also has good properties. CTL (coal to liquid) and GTL (gas to liquid) are established industries, and there is a large and growing interest in developing BTL (biomass to liquid) processes. Large scale BTL will probably utilize entrained flow gasification, where the biomass is converted to syngas at temperatures above slagging (ash melting point). Thus, issues with ash components need to be resolved in order to protect downstream catalysts and processes. Alkali and alkaline earth metals represent an important part of produced ash particulates because of their strong negative effect on catalyst activity.

Previous work in this group and by others investigated the influence of alkali metals using a simplified method of deposition based on the incipient wetness impregnation technique. The purpose of this project is to verify the validity of these results through a gas phase deposition route, and also to improve the understanding of how the alkali (potassium specifically) influences a Co-based F-T catalyst. We have adapted an aerosol deposition technique, inspired by similar work on a Ni catalyst in the SCR reaction. The aerosol could better represent in situ poisoning and therefore give a more realistic picture of the effect of potassium. This knowledge will be useful for designing new BTL plants.

Potassium salts were deposited using aerosol deposition on a 20%Co/0.5%Re/γAl_2O_3 catalyst. Potassium salts are dissolved in deionized water and the solution is placed inside an "atomizer", which produces aerosol particles. Nitrogen is used as a carrier gas which forces aerosol particles in the reactor direction and through the catalyst bed. The catalyst bed is placed in a reactor which can be heated up to 300°C.

The characterization showed that the poisoned catalysts have the same dispersion, surface areas and reduction peaks as the unpoisoned one, independent of the level of potassium, up to around 3500 ppm. This is in agreement with previous work where impregnation using water as the solvent was used as method of deposition. However, activity results showed a dramatic drop in catalyst activity, measured as STY (site time yield), with increasing potassium level. Product selectivity was affected only slightly with increasing potassium concentration. It was previously discussed that mobility of potassium might play a role during the catalyst deactivation, and our results do not disagree with this idea. Characterization of the produced aerosol particles showed that their particle size is much larger than the catalyst pores, so this indicates that the potassium probably moves to specific sites on the cobalt surface related to the Fischer-Tropsch synthesis activity during pretreatment or reaction.

Financial support:
The Research council of Norway, ENERGIX programme (contract no: 228741)

Collaboration: Linnaeus University, Växjø, Sweden

Presentations in 2016:
Ljubiša Gavrilović, Edd A. Blekkan, Anders Holmen, Hilde J. Venvik, R. Myrstad, Jan Brandin, *Influence of potassium species on Co based Fischer-Tropsch catalyst.* The 11th Natural Gas Conversion Symposium (NGCS 11), Tromsø, Norway. 5 - 9 June, 2016.

Material degradation by metal dusting corrosion on instrumentation used in micro-structured reactors

Ph.D. Candidate: Xiaoyang Guo
Supervisor: Prof. Hilde Johnsen Venvik
Co-supervisors: Senior Scientist John Walmsley, Assoc. Prof. Estelle Vanhaecke, Postdoctoral Fellow Daham Gunawardana and Prof. De Chen.

Metal dusting is a corrosive degradation phenomenon on metals and alloys that proceeds by a gradual breakdown of the material into fine particles. It constitutes a problem in the chemical industries, where metals and alloys are extensively exposed to carbon-supersaturated gaseous with low partial pressures of oxygen and/or steam in a critical temperature range of 300–850 ˚C. Metal dusting carries significant cost, since certain precautions need to be taken to avoid catastrophic events in these processes. Microstructured reactors are being developed for process intensification in order to enable safer, more cost-effective and sustainable conversion of natural gas in the small-to-medium scale. Due to the large inner surface area of the reaction volumes and highly integrated heat exchange between reactant and product streams, metal dusting becomes an even more severe issue.

In this study, we are focusing on understanding the metal dusting mechanism and identifying possible controlling variables in view of compact technology for generation and conversion of syngas. Fe- and Ni-based (Incoloy 800 and Inconel 601) industrial alloy samples were pre-oxidized in 10% steam in Ar at 540 ˚C for 6h, followed by exposure to reducing, highly carburizing atmosphere. Several carburizing parameters were studied, such as the temperature (550, 650, 750 ˚C) and the pressure (1 bar or 20bar). Two carburizing gas mixtures were used: a CO +Ar mixture with 10/90(mol %) composition ratio, and a CO/H2O/ CO2/H2/Ar mixture with 20/10/15/25/30 (mol%) composition ratio to mimic industrially

relevant synthesis gas. Length of exposure time was also varied from 1 h to 20h. The resulting surfaces were examined by using Raman spectroscopy, scanning electron microscopy (SEM), depth profile analysis by Auger electron spectroscopy (AES) under ion-sputtering and transmission electron microscopy (TEM).

As indicated by electron microscopy, Alloy 800 samples treated under CO+Ar at low temperature and low pressure (i.e. 550 ˚C and 1 bar) showed a thick layer of surface carbon deposits. The amount of carbon formed on Inconel 601 and on Incoloy 800 is clearly a function of exposure temperature and time as well the gas composition. Increase of exposure temperature under CO-Ar gas lowers the carbon formation. This requires further investigation in view of the infinite carbon activity and presumed kinetic control under such conditions. Existence of carbon formation could so far not be confirmed under the syngas mixture, irrespective of the exposure temperature and pressure, and this is in partial contrast to our previous investigations of Inconel 601. The surface oxide layer formed in Incoloy 800 hence shows better performance under CO-Ar conditions than that of Inconel 601, but further investigations are required. FIB cross-section analysis shows interesting details of the chromium oxide rich surface oxide layer. The short exposure alloy 601 samples (1-2h) show that carbon formation is induced in the early stage of the exposure. Further characterization of these samples aims at establishing a link between the surface structure and composition and the initiation of the carbon growth.

Financial support:
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Presentation in 2016:
Xiaoyang. Guo, P.V.D.S. Gunawardana, Estelle M. M. Vanhaecke, Jihye Hwang, John Walmsley, De Chen and Hilde J. Venvik, Material degradation by metal dusting corrosion on instrumentation used in natural gas conversion technologies, NGCS 11 --11th Natural Gas Conversion Symposium. Tromsø Norway 6 – 9 June 2016, Poster

Kinetic Study of Bimetallic Catalysts for Compact Steam Reformer

Ph.D. Candidate: Shirley Elisabeth Liland
Supervisor: Prof. De Chen
Co-supervisor: Dr. Kumar Ranjan Rout

Today the preferred route to chemicals and liquid fuels are through synthesis gas, where synthesis gas production accounts for at least 60% of the total plant investment. The production is most commonly performed by the steam reforming (SR) process. A possibility for reducing the costs will be to achieve a small scale GTL (Gas to liquid) process using a microchannel reactor.

The goal for this project is to develop a new microchannel reactor to achieve the maximum volumetric productivity. This will be accomplished through optimization of the integration of combustion and steam reforming processes, including development of advanced catalysts for both processes. Reactor modeling and analysis will be utilized to analyze how to achieve the maximum heat flux between the two adjunct channels, which will limit the maximum reaction rate of steam reforming. An advantage of the microchannel reactor is that it can be further integrated into compact Fischer-Tropsch reactors. In the microchannel reactor the SR reaction

(endothermic, outer channel) will get energy supplied as heat from a combustion reaction (exothermic, inner channel).

There are two catalysts needed for this reactor, one for each reaction. For the SR reaction a bimetallic Ni based catalyst supported on a hydrotalcite-like structure will be the main focus. There has already been performed several studies on different catalytic metals for steam reforming, including bimetallic Ni catalysts. However not much attention has been given to the compact reformer, which means there are many aspects of the catalytic compact reformer that still needs to be investigated. The same catalysts will be investigated for the combustion reaction, as we believe these are also active for the methane decomposition.

The end goal for this project is to collect information that will lead to more attractive investments in industrial processing of natural gas in Norway.

Presentations in 2016

1. Dam, A.H.; Wang, H.; Liland, S.E.; Holmen, A.; Chen, D., *The methane adsorption activation energy dependency on different three-hollow sites*. Oral presentation at The 11th Natural Gas Conversion Symposium; June 05-09 (2016) Tromsø, Norway
2. Liland, S.E.; Yousaf, B.; Rout, K.R.; Wang, Y.; Chen, D., *Unprecedented Active and Stable Ni-Co Bimetallic Catalyst for Steam Methane Reforming*. Poster at the 16th International Congress on Catalysis; July 03-08 (2016), Beijing, China

Financial support:
The project is funded by the Research Council of Norway under the GASSMAKS research program (Project 233869)

Metal dusting corrosion initiation on the surface of INCONEL® 601 **alloy**

Postdoctoral Fellow: Dr. Daham S. Gunawardana Panditha Vidana
Supervisor: Prof. Hilde Venvik

Metal dusting is a catastrophic corrosion degradation process in which metallic materials disintegrate into dust of fine metals and metal oxide particles mixed with carbon. It is a costly issue in petrochemical and syngas technologies, where metals and alloys are exposed to carbon-saturated gaseous environment with low oxygen/steam partial pressures (carbon activity, $a_C > 1$) at temperatures above 400 ˚C. The overall objective of this study is to advance the understanding of the early stage in metal dusting corrosion, *i.e.* the initiation of the carbon formation and role of the composition and structure of the surface oxide layer in this respect. In general, the initial phase of carbon formation and the progress of the metal dusting in the alloy matrix are affected by wide range of micro- and macro-scale parameters; including material stresses, diffusivity of metal components, grain orientation and reaction kinetics as well as gas flow rate, temperature, pressure, gas composition and exposure time. Great care has therefore been taken to develop experimental protocols that are consistent and application relevant.

The projects is a continuation of PhD research, in which surface polished coupon-like Ni-based industrial alloy (INCONEL® 601) samples were first subjected to oxidation treatment at different temperatures (540, 760 or 980 ˚C) in gas atmospheres with different steam or oxygen partial pressures (P_{O_2}). The pre-oxidized samples were then exposed to different

syngas atmospheres with either *infinite* or *finite* carbon activity ($a_C >> 1$ or $a_C > 1$). The resulting surfaces and carbonaceous products were characterized by means of optical microscopy, electron microscopy (both SEM and TEM) in conjunction with EDS, AES under ion-sputtering and XPS.

Financial support:
The Research Council of Norway; Statoil, INEOS and Haldor Topsøe AS through the project Innovative Natural Gas Processes and Products (*in*GAP).

Improving the Performance of Existing Formalin Production Process Technology

Ph.D. Candidate: Stine Lervold
Supervisor: Prof. Hilde J. Venvik
Co-supervisor: Assoc. Prof. Jia Yang and Senior Researcher Dr.ing Rune Lødeng.

Formaldehyde is the essential component of wood adhesives for a wide range of applications and an important intermediate in the production of several fine chemicals. Formaldehyde is produced via selective catalytic oxidation of methanol to formaldehyde. Industrially production of formaldehyde from methanol is performed via two main processes: partial oxidation over a silver catalyst or by oxidation in excess air over base metal oxides. Dynea owns both technologies, and recognizes an economic potential for the silver-based process with the main objective to improve yield and lifetime of the silver catalyst.
The PhD project focuses on specific kinetic experiments and linking these to the structure/composition of the Ag catalyst. An initial activity concerns development of experimental protocols that allow extraction of kinetic data in an experimental setup, including specific reactor designs. Parameters affecting the selectivity and stability of Ag will be studied by investigating surface and bulk structural properties and how these develop with time on stream. This approach seeks to identify the effect of reaction conditions on structural properties. In addition, understanding the role of (surface) AgOx species by utilization of advanced characterization and microkinetic modelling.
Investigation of both chemical and kinetic aspects will be performed in a so-called annular reactor. The annular reactor offers a controlled system with laminar flow, isotherm conditions and potentially negligible mass transport limitations and gas phase reactions.

Presentations in 2016:
Stine Lervold, Jia Yang, Rune Lødeng, Kristin Bingen, Terje Pedersen, Hilde J. Venvik. *Establishing Experimental Methodology for Silver Catalyst in Formaldehyde Synthesis*. iCSI Kick off Seminar, Trondheim, Norway, 2016. Poster presentation.

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Biomass derived Fe/N/P tridoped carbon electrocatalysts for oxygen reduction reaction and zinc-air batteries

Ph.D. Candidate: Yahao Li
Supervisor: Prof. De Chen

In order to mitigate global warming, tremendous efforts have been dedicated to reduce the greenhouse gases emission. To utilize clean energy such as electricity instead of fossil fuel is one of the major attempts. Within all electric devices, metal-air battery is attractive for its high energy density, high capacity and low fabrication cost. To fabricate a high quality metal-air battery, an efficient catalyst for oxygen reduction reaction (ORR) is essential. Platinum (Pt) base catalysts, including Pt alloy, are by far the most efficient among all catalysts. However, as one of the noble metal, the lack of abundance of Pt lead to the high cost, which hinders its commercial applications. Recent studies revealed that nitrogen doped carbon nanomaterials possess impressive ORR activities, and co-doping phosphorus into the materials can further enhance the ORR activity due to the modulation of electronic properties and surface polarities. Meanwhile, carbon supported iron-nitrogen complexes Fe-N_x were also believed to be an effective active site for ORR. Both strategies can lead to excellent electrocatalysts, and combining them together may result even better catalysts.
We used a simple one-step procedure to fabricate Fe/N/P tridoped biomass derived carbon materials (Fe-N-P-C) and tested the activities towards oxygen reduction. Fe-N-P-C possesses a mesoporous structure with high specific surface area of around 1500 m^2/g and excellent ORR activities of onset and half-wave potential of 1.050 V and 0.874 V (vs. RHE) that even surpass the performance of 30 % Pt/C catalyst. While utilized as air-electrode in Zn-air battery, gorgeous performances of open-circuit potential of 1.48 V, an energy density of 771 Wh/kg_{Zn} and a peak power density of 100 mW/cm^2 were also achieved.

Financial support:
The project is funded by Chinese Scholarship Council.

Integrated *H_2BioOil* process for efficient biofuel production

Postdoctoral Fellow: Dr. María Victoria Gil Matellanes
Supervisor: Prof. De Chen

The access to clean and sustainable energy is currently an important challenge. The growing global concern about climate change and CO_2 emissions to the atmosphere requires the research and development of new energy generation technologies from renewable sources, such as biomass. The aim of this project is to provide experimental proof of an integrated *H_2BioOil* process for fully sustainable production of biofuels from lignocellulosic biomass.

The integrated process includes high pressure fast-hydropyrolysis (FHP) of wood biomass powders for producing hydrogen, followed by an immediate downstream vapor-phase catalytic aldol-condensation (CAC) and catalytic hydrodeoxygenation (HDO) to produce hydrocarbon products (C_4-C_{16+}). The system is also integrated with pressure swing sorption enhanced steam reforming (SESR) of the byproducts from the process to produce hydrogen at high pressure. This is a novel process with high fuel yield and energy efficiency, and it represents a fully sustainable process of hydrogen generation from biomass. The global

goal of the project is to provide the experimental proof-of-concept for sustainable production of drop-in transportation fuels from biomass.

Fast-hydropyrolysis involves a rapid heating of biomass up to temperatures of about 500 ºC in a high pressure hydrogen environment to produce vapors, which sequentially will be catalytically aldol-condensed/ketonizated and hydrodeoxygenated to produce hydrocarbon products (C_4-C_{16+} and C_1-C_3), CO, CO_2, H_2 and H_2O. These products, except C_4-C_{16+}, will be treated by sorption enhanced steam reforming to produce H_2, which will be integrated in the FHP reactor. In the SESR process, a high-temperature CO_2 sorbent, Arctic dolomite, is incorporated into the catalyst bed to in situ remove the carbon dioxide from the gaseous phase. Hence, the thermodynamic equilibrium limits of the reversible reforming and water gas shift (WGS) reactions are shifted towards the hydrogen production, so obtaining a high hydrogen conversion in a single step.

Publications and presentations in 2016:

1. Gil, María Victoria; Fermoso, Javier; Pevida, Covadonga; Chen, De; Rubiera, Fernando. *Production of fuel-cell grade H_2 by sorption enhanced steam reforming of acetic acid as a model compound of biomass-derived bio-oil.* Applied Catalysis B: Environmental 2016; Volum 184. s. 64-76.
2. Esteban-Díez, Gonzalo; Gil, María Victoria; Pevida, Covadonga; Chen, De; Rubiera, Fernando. *Effect of operating conditions on the sorption enhanced steam reforming of blends of acetic acid and acetone as bio-oil model compounds.* Applied Energy 2016; Volum 177. s. 579-590.
3. Gil, María Victoria; Esteban-Díez, Gonzalo; Pevida, Covadonga; Rubiera, Fernando; Chen, De. *H_2 production by sorption enhanced steam reforming of biomass-derived bio-oil.* Poster presentation, 11th Natural Gas Conversion Symposium (NGCS11), Tromsø (Norway), 5-9 June 2016.

Financial support:
The project is funded by the Research Council of Norway (NFR) through the ENERGIX programme.

Methane dry (CO_2) reforming on Ni@Pt catalysts studied by experiment and DFT

Ph.D. Candidate: Juntian Niu
Supervisor: Prof. De Chen, Department of Chemical Engineering, NTNU
Co-Supervisor: Jingyu Ran, College of Power Engineering, Chongqing University

Methane dry (CO_2) reforming is a promising reaction that is of both scientific and industrial importance. Ni was widely applied in this process because of low cost compared with noble metal catalysts, however, single component Ni catalysts are not able to meet the activity, selectivity and stability requirements. Pt-Ni bimetallic catalysts show the good performance for carbon resistance, activity and stability from both the experimental and theoretical studies in methane oxidation and reforming.

In this project, my work focuses the synthesis of monometallic Ni catalyst derived from hydrotalcite-like precursor and preparation of bimetallic Ni@Pt catalysts based on redox

reaction. The physical-chemical properties of the catalysts were investigated by N_2 physisorption, H_2 chemisorption, X-ray diffraction (XRD), H_2 temperature programmed reduction (H_2-TPR), X-ray fluorescence (XRF), X-ray photoelectron spectroscopy (XPS) and transmission electron microscopy (TEM). Catalytic tests for methane dry reforming focus on the activity at different temperature, stability after a period experimental operation and selectivity for H_2 and CO. In addition, with the Pt loading increase on the surface of Ni catalysts, the behavior for coke formation and ability to anti-carbon deposition have been discussed to shed some light on coke mechanism on monometallic Ni/Mg(Al)O catalyst and the role of Pt in coke elimination. In addition, according to DFT computational work, the energy barrier for CH dissociation on Ni@Pt(111) core-shell surface is remarkably increased by around 1.979 eV and the carbon adsorption energy is lower compared to those on Ni(111) and Pt(111). These results are helpful to understand the mechanisms of methane oxidation and reforming from the atomic scale.

Financial support: China Scholarship Council (Grant No. 201606050054).

Fundamental understanding of Fe and Co based catalysts for light olefin production via the direct Fischer-Tropsch to olefins (FTO) process

Ph.D. Candidate: Eirik Østbye Pedersen
Supervisors: Prof. Edd A. Blekkan, Prof. De Chen.

Fischer-Tropsch synthesis (FTS) is mainly used for production of longer alkanes for fuel use, and has been subject to thorough research throughout the 20th century. More recent research works show that high selectivity for light (C_2-C_4) olefins is obtainable with tailored catalysts using the right combination of active metals, supports and promoters as well as operating conditions. Light olefins are among the most important chemical intermediates on the market and the FTO process is considered an attractive future method of light olefin production from natural gas.

This project aims at obtaining a better understanding of chain growth and termination in the FTO process as a function of catalyst properties. The work applies a multiscale approach, integrating first principles calculations (DFT), and advanced catalyst preparation, characterization and testing methods.

Manganese is considered an important promoter for increasing light olefin selectivity in the Fischer-Tropsch process. FTS over Mn-promoted Co/Al_2O_3 catalysts is investigated by combining experimental and theoretical methods.

The effect of Mn promotion on Co catalysts is investigated by varying catalyst preparation method and reduction conditions. The state of Mn and its effect on Co is investigated using *in situ* characterization techniques such as XANES and XRPD under relevant reaction conditions and the role of Mn in H_2 and CO adsorption on Co will be investigated using SSITKA, Raman, TPD and XPS.

The promotion effects of Mn on Co is also investigated by DFT. Calculations focus on the effect of Mn addition on the adsorption energies of relevant species on Co as well as the dissociation of CO, the formation of CH_4 and the formation and desorption of light olefins. The structure and promotion effect of MnO will be investigated, in particular the role of the Co-MnO interface.

Presentations in 2016:

1. Østbye Pedersen, Eirik; Svenum, Ingeborg-Helene; Blekkan, Edd. A. *Co-Mn Catalysts for Fischer-Tropsch Production of Light Olefins*. Oral presentation, 11th Natural Gas Conversion Symposium; 5.6.2016-9.6.2016, Tromsø, Norway.

2. Østbye Pedersen, Eirik; Svenum, Ingeborg-Helene; Blekkan, Edd. A. *Co-Mn Catalysts for Fischer-Tropsch Production of Light Olefins*. Poster presentation, 11th Natural Gas Conversion Symposium; 5.6.2016-9.6.2016, Tromsø, Norway.

Funding:
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Reaction mechanism investigation by combined DFT calculations and microkinetic modelling

Postdoctoral Fellow: Dr. Yanying Qi
Supervisor: Prof. De Chen

Density functional theory (DFT) calculations can be used to describe surface reactions and provide the descriptors of catalytic activity and selectivity to be able to tailor catalysts atom by atom. Microkinetic modelling is utilized to investigate the reaction mechanism and predict information about surface coverages under reaction conditions and relative rates of various elementary steps. A schematic figure of DFT based microkinetic modelling is shown in Figure.1. By using this methodology, we could predict the kinetic behavior based on DFT calculations, which will bridge the gap from DFT calculations at atomic level to kinetic analysis at macro-scale. This will be employed to reaction systems of vinyl chloride monomer synthesis and formaldehyde synthesis.

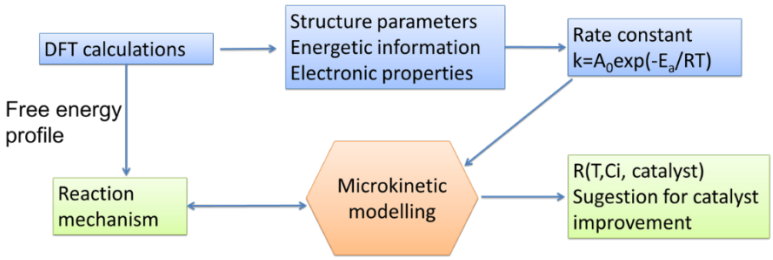

Figure 1. Schematic figure of DFT-based microkinetic modelling

The partial oxidation of methanol to formaldehyde is an important industrial process due to the versatility of formaldehyde as an intermediate in chemical synthesis. I did a literature review of the DFT calculations of Ag-catalyzed methanol oxidation process in order to explain the experimental results. Based on the references, it is found that water is easily to dissociate to generate OH and O, which could inhibit the decomposition of formaldehyde. This may explain water in the feed seems to improve selectivity. The oxygen dissociation is suggested to be the rate determining step by a degree of rate control analysis form one reference, which may be a reason for the activation energy similar to diffusion of oxygen in silver.

Catalytic oxychlorination of ethylene with hydrochloric acid and oxygen is one of the most important routes to produce 1, 2-dichloroethane (EDC), a key intermediate in polyvinyl chloride (PVC) production. The previous work found that alkali metals, such as K, Na, and/or rare earth metals like La as promoters increase the activity-, selectivity- and stability of $CuCl_2$ based catalysts by kinetic studies. However, the underlying mechanism of promoter effect is not fully understood. We are beginning to study the promoter effect by DFT calculations.

Financial support:
The project is a research activity under iCSI – industrial Catalysis Science and Innovation for a competitive and sustainable process industry", which is a National Centre for Research-based Innovation (SFI) granted by the Research Council of Norway.

Advanced *in situ* characterization of catalysts for sustainable process industry

Ph.D. Candidate: Samuel K. Regli
Supervisor: Prof. Magnus Rønning
Co-Supervisor: Prof. Hilde J. Venvik

This PhD project is part of the industrial Catalysis Science and Innovation (iCSI) Centre, a national center for research-based innovation. Industrial chemical processing and energy conversion continuously needs to be improved for minimum environmental impact and sustainability, requiring a detailed understanding of the kinetics and chemistry involved. The industrial partners involved supply key sectors of the global market (catalysts, chemicals, fertilizer, plastics, fuels, etc.).

Heterogeneous catalytic systems are complex and a simplification is often not adequate at industrial conditions, hence an experimental mode combining both the acquisition of kinetic and structural information in the same setup, called *in situ* or *operando*, is required. Such an approach could bring more mechanistic insights to the kinetic modelling and subsequently make more accurate predictions of the relevant kinetic steps. Moreover, the combined approach could significantly improve the parameter reliability by direct measurement of adsorption parameters in kinetic models.

The project will focus on *in situ* characterization of catalysts for the following three iCSI industrial processes:

- 21^{st} century Ammonia oxidation and Nitric acid technology development
- Frontier formalin technology development
- PVC value chain: World class energy and raw material efficiency for the production of Chlorine and Vinyl Chloride Monomer (VCM)

The key characterization techniques in this project – X-ray absorption spectroscopy and X-ray diffraction with synchrotron radiation, Fourier-transform infrared spectroscopy and Raman spectroscopy – can be readily combined for measurements of the bulk and surface of the catalyst simultaneously during operation at industrially relevant temperatures (473-723 K) and pressures (up to 20 bar).

New insight on the active sites of the catalysts and the respective kinetics of the chemical reactions can guide towards favorable compositions and conditions enabling processes with higher efficiency, lower energy consumption and improved lifetime.

Financial support:
The project is a research activity under iCSI – industrial Catalysis Science and Innovation for a competitive and sustainable process industry", which is a National Centre for Research-based Innovation (SFI) granted by the Research Council of Norway.

Poster presentation in 2016:
Regli SK, Rønning M. *Advanced in situ characterization of catalysts for sustainable process industry*. Industrial Catalysis Science and Innovation Kick-off Seminar, November 2016, Trondheim, Norway.

Conversion of biomass to transportation fuels

Ph.D. Candidate: Haakon Rui
Supervisor: Prof. De Chen
Co-Supervisor: Prof. Edd Blekkan

The hydrogenolysis of cellulose into different products is a very interesting topic, with many articles already published. The hydrogenolysis of cellulose can provide e.g. alcohols, diols and 5-hydroxymethylfurfural (5-HMF) depending on the reaction conditions. Currently, investigations are being done employing a Ru/CNT catalyst together with tungstic acid (H_2WO_4), which results in yields of roughly 60% ethylene glycol (EG) and 10% propylene glycol (PG) from the cellulose hydrogenolysis. The particle size effect of the active metal catalyst for this reaction system is being investigated, as early studies have shown that a lower loading of ruthenium gives a higher yield of products at the same Ru:W molar ratio. Ideally, a descriptor for the selectivity of the products, especially in regards to the EG/PG yield, would be found. A range of different solid bases and acids have been tested for this reaction, but none have been close to achieving the same results as for the Ru/CNT+H_2WO_4 system. The effect of employing different CNT-supported metals (nickel, copper etc) and additives (e.g. H_2SO_4) is next in line to be studied. The primary goal is to achieve a high selectivity of C2, C3, C4 or C6 diols respectively, and thereafter upgrading these into fuel additives via aldol-condensation. Aldol-condensation of PG has already been done by another group here at IKP.

Financial Support:
The PhD project is a part of the Nordic Five Tech (N5T) graduate school in Thermal and Catalytic Conversion of fuels (http://www.nordicfivetech.org/).

Catalysts for attaining NO/NO_2 equilibrium

Ph.D. Candidate: Ata ul Rauf Salman
Postdoctoral Fellow: Xavier Auray
Supervisor: Prof. Magnus Rønning,
Co-supervisors: Senior Scientists Rune Lødeng and Bjørn Christian Enger

Nitric acid is an important industrial chemical. Commercial production of nitric acid takes place via the Ostwald process. The process comprises of three steps

1. Oxidation of ammonia with atmospheric oxygen to produce nitric oxide

$$4NH_3 + 5\,O_2 \longrightarrow 4\,NO + 6\,H_2O \qquad \Delta Hr_{298} = -907\ kJ/mol$$

The reaction is catalyzed by Pt-Rh gauzes. Typical concentrations at the exit of ammonia combustor are NO (10%) and H_2O (15%).

2. Oxidation of the nitric oxide to nitrogen dioxide

$$2\,NO + O_2 \longrightarrow 2\,NO_2 \qquad \Delta Hr_{298} = -113.8\ kJ/mol$$

The oxidation of nitric oxide is a homogenous gas phase reaction occurring in the waste heat boiler, enabling heat recovery.

3. Absorption of the nitrogen dioxide in water to form nitric acid

$$3\,NO_2 + 2\,H_2O \longrightarrow 2\,HNO_3 + NO \qquad \Delta Hr_{298} = -37 kJ/mol$$

The objective of the project is to develop an active catalyst to fully oxidize NO to NO_2 in step 2. The catalyst will help to reduce the capital investment by replacing the bulky homogeneous oxidation process by compact heterogeneously catalyzed process. A catalyst working at 300^{o}C has the potential of 15 % additional heat recovery from the NO oxidation process.

An experimental setup capable of testing catalyst for NO oxidation under industrial conditions was designed and built. NO oxidation has been investigated both with and without catalyst. Pt/Al_2O_3 catalyst, prepared by incipient wetness impregnation, was chosen as a reference catalyst. Catalyst activity and stability was investigated under different NO concentrations (ranging from typical dilute diesel oxidation conditions to concentrated nitric acid plant compositions), flowrates and temperatures. The catalysts have been characterized by H_2 and CO chemisorption, XRF, TPR and BET. The Pt/Al_2O_3 catalyst shows promising activity towards oxidation of NO under industrial conditions.

Financial Support:
The project is a research activity under iCSI – industrial Catalysis Science and Innovation for a competitive and sustainable process industry", which is a National Centre for Research-based Innovation (SFI) granted by the Research Council of Norway.

Surface science investigations of model systems for Co and Pd based catalysts

Ph.D. Candidate: Marie D. Strømsheim
Supervisor: Prof. Hilde Johnsen Venvik
Co-supervisors: Prof. Anne Borg, Department of Physics, NTNU, and Research Scientist Dr. Ingeborg-Helene Svenum, SINTEF

Single crystals provide model systems that can further the understanding of phenomena occuring at the surface of a catalyst e.g adsorption/desorption, restructuring, reaction, surface segregation, promotion and poisoning. The surface of Co(11-20) represents a model system for cobalt (Co) based Fischer – Tropsch (FTS) catalysts for conversion of synthesis gas derived from natural gas or biomass into liqiuid fuels. Previous experiments by Lillebø et al. and Patanou et al. at KinCat reported a significant decrease in the catalytic activity for Co-based catalysts with added small alkali metal impurity loadings (up to 1000 ppm). However, the H_2 chemisorption properties and the H_2 and CO differential heats of adsorption remained unaffected. Therefore, the deposition of submonolayer amounts of potassium (K) on Co(11-20), and its effect on FTS relevant adsorption phenomena were studied using various surface science techniques; Low Energy Electron Diffraction (LEED), Scanning Tunneling Microscopy (STM), and High resolution x-ray photoelectron spectroscopy (HRXPS). Density functional theory (DFT) calculations of the Co(11-20) surface were also performed to complement the experimental results. Previous STM investigations, performed by the group, have shown that adsorption of CO ($1\text{-}3\cdot10^{-9}$ mbar) at room temperature on clean Co(11-20) induces a (3x1)-reconstruction of the surface that involves anisotropic transport of Co from and to the step edges. The (11-20) orientation was therefore chosen as a model system for the investigation of surface restructuring upon exposure to FTS relevant adsorbates. Performing a similar experiment with pre-deposited submonolayer amounts of K on the surface, showed notable differences in the reconstruction process and resulted in a surface with a higher degree of disorder in STM. Measurements with HRXPS at ASTRIDII in Aarhus, Denmark of the adsorption of CO on Co(11-20) with and without predeposited submonolayer amounts of K demonstrated that small amounts of K resulted in a significant reduction in the amount of CO adsorbed.

Palladium (Pd) based catalysts are often applied in oxidation and hydrogenation reactions. Alloying elements such as Ag, Cu and Au may affect the nature of the reactive surface, the stability, or provide a reduction in the noble metal cost. The formation of ordered oxides on Pd and Pd alloy single crystals has been shown to affect the catalytic performance in oxidation reactions. A $(\sqrt{5}\times\sqrt{5})R27°$ surface oxide has been observed on $Pd_3Au(100)$, under ultra-high vacuum (UHV) conditions, similar to Pd(100) and $Pd_{75}Ag_{25}(100)$, formed upon oxygen exposure of $\sim10^{-3}$ mbar, and ~310 °C. To further elucidate the effect of Au as an alloying element, CO oxidation over $Pd_3Au(100)$ was studied with Near Ambient Pressure XPS (NAPXPS) and quadropole mass spectroscopy (QMS) at the SPECIES beamline at the MAXIV Laboratory in Lund, Sweden, under oxygen rich conditions (O_2:CO=10:1), and ~1 mbar total pressure. The QMS data showed that the $Pd_3Au(100)$ surface is active towards CO_2 formation above ~190 °C, above which the reaction becomes mass transfer limited. Moreover, the Pd 3d and O 1s core level spectra are consistent with the $\sqrt{5}$ oxide being present in the region of high catalytic activity, which is also the case for Pd(100) but not $Pd_{75}Ag_{25}(100)$, where chemisorbed oxygen constituted the active phase. Furthermore, $Pd_3Au(100)$ does not display reversed hysteresis, i.e. cycling dependency of the activity with temperature, which was the case for $Pd_{75}Ag_{25}(100)$.

Financial support:
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The computations were performed on resources provided by UNINETT Sigma2 - the National Infrastructure for High Performance Computing and Data Storage in Norway, account no. NN9152k and NN4654k.

Publications and presentations in 2016:

1. Marie. D. Strømsheim, Ingeborg-Helene Svenum, Ljubisa Gavrilovic, Xiaoyang Guo, Mari H. Farstad, Anne Borg, Hilde J. Venvik. *Co single crystal surfaces as Fischer-Tropsch model systems: STM investigations of alkali metal on Co single crystal surface"*. Oral presentation at The 11th Natural Gas Conversion Symposium (NGCS11), Tromsø, Norway, (05.06.2016-09.06.2016)

2. Marie. D. Strømsheim, Jan Knudsen, Xiaoyang Guo, Linn C. Sørvik, Vasco R. Fernandes, Hilde J. Venvik, Anne Borg, *Near ambient pressure XPS investigation of CO oxidation over $Pd_3Au(100)$*, Oral presentation at The 17th Nordic Symposium in Catalysis (NSC17), (14.06.2016-16.06.2016).

3. Marie D. Strømsheim, Jan Knudsen, Mari H.Farstad, Linn Sørvik, Xiaoyang Guo, Hilde J. Venvik, and Anne Borg. *Near ambient pressure XPS investigation of CO oxidation over Pd3Au(100)* Accepted for publication in *Topics in Catalysis*

4. Marie D. Strømsheim, Ingeborg-Helene Svenum, Mari H. Farstad, Zheshen Li, Ljubisa Gavrilovic, Xiaoyang Guo, Stine Lervold, Anne Borg, and Hilde J. Venvik. *Effects of K adsorption on the CO-induced restructuring of Co(11-20).* Submitted to *Catalysis Today*

Structure - performance relations of Co-based Fischer – Tropsch synthesis catalysts

Postdoctoral Fellow: Dr. Nikolaos Tsakoumis
Supervisor: Prof. Magnus Rønning
Co-supervisors: Prof. Anders Holmen, Prof. II Erling Rytter.

The Fischer-Tropsch synthesis (FTS) is an important part of most natural gas conversion (GTL) process developments in recent years. Modern Fischer-Tropsch synthesis aims at converting synthesis gas into high quality diesel. A key element in improved Fischer-Tropsch technology is the development of active and stable catalysts with high wax selectivity. Cobalt is considered the most favourable metal for the synthesis of long-chain hydrocarbons.

As in any other investigation of catalytic materials, unravelling structure - performance relations is important for the understanding the catalytic processes itself. Co-based FTS is a structure sensitive reaction where the cobalt particle size and phase, in addition to effects from the used support and promotor, are interplay. The high complexity of the

reaction dictates that a detailed examination of the catalytic material has to be performed and therefore catalyst characterisation in all the stages of catalyst lifetime is crusial.

The current project aims in the study of catalytic behaviour of FTS catalysts modified in different ways towards better understanding of structure – selectivity relations. Catalyst activity, selectivity and stability will be evaluated in a rig with 4 fixed-bed reactors connected in a parallel configuration. Different characterization techniques will be applied in all stages of the experimental procedure in order to unravel the bulk and surface composition of the active phase as well as the support. The preferred characterization techniques that will be on focus are X-ray absorption spectroscopy (XAS), X-ray powder diffraction (XRPD), Raman and IR spectroscopies, H_2 chemisorption and Transmission electron microscopy (TEM).

Publications and presentations in 2016:

1. E. Rytter, A. R. Salman, N.E. Tsakoumis, R. Myrstad, J. Yang, S. Lögdberg, A. Holmen and M. Rønning, Hydrophobic Catalyst Support Surfaces by Silylation of γ-Alumina for Co/Re Fischer-Tropsch Synthesis, (**2016**) *Submitted*.
2. E. Patanou, N.E. Tsakoumis, R. Myrstad, E. A. Blekkan, The impact of sequential H_2-CO-H_2 activation treatment on the structure and performance of cobalt based catalysts for the Fischer-Tropsch synthesis (**2016**) *Submitted*.
3. N.E. Tsakoumis, J. C. Walmsley, M. Rønning, W. van Beek, E. Rytter, A. Holmen, Evaluation of reoxidation thresholds for γ-Al_2O_3 supported cobalt catalysts under Fischer - Tropsch synthesis conditions**,** *J. Am. Chem. Soc.* (**2016**), *Accepted*.
4. C. Sprung, E.A. Redekop, R.D. Armstrong, N.E. Tsakoumis, Midnight-sun-induced natural gas conversion, Catal. Today (**2016**) *Accepted*.
5. N.E. Tsakoumis, R. Johnsen, W. van Beek, M. Rønning, E. Rytter, A. Holmen, Capturing metal-support interactions in situ during the reduction of a Re promoted Co/γ-Al_2O_3 catalyst. *Chem. Commun*. 52 (**2016**) 3239-3242. **(*Highlighted at 2015-2016 biannual report of the Swiss-Norwegian beamlines @ESRF*).**
6. E. Rytter, N.E. Tsakoumis, A. Holmen, On the selectivity to higher hydrocarbons in Co-based Fischer–Tropsch synthesis, *Catalysis Today* 261 (**2016**) 3-16. ***(in the Top 25 hottest articles of "Catalysis Today").***
7. N.E. Tsakoumis, M. Rønning, E. Rytter, A. Holmen. *Utilization of synchrotron X-rays for studying the state of catalysts during a chemical process; the case study of Co-based Fischer – Tropsch synthesis.* Oral presentation, 17th Nordic Symposium on Catalysis. Lund, Sweden, 14 – 16 June 2016.
8. N.E. Tsakoumis, M. Rønning, E. Rytter, A. Holmen. *In situ monitoring of supported cobalt catalysts for Fischer-Tropsch synthesis under realistic conditions; what have we learned?* Oral presentation, 11th Natural Gas Conversion Symposium Gas Conversion (NGCS). Tromsø, Norway, 05 – 09 June 2016.

Financial support:

The work is financed by Statoil and the Norwegian Research Council through the *in*GAP project (Innovative Natural Gas Processes and Products).

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

NTNU: Postdoctoral Fellow Eleni Patanou, Postdoctoral Fellow Nikolaos Tsakoumis, Prof. Edd A. Blekkan
SINTEF: Research Scientist Rune Myrstad

Fischer – Tropsch synthesis (FTS) is the heart of Gas-to-Liquids process for the utilization of synthesis gas derived from natural gas. In the Co-based FTS two types of reactors are dominant, the multi-tubular fixed-bed reactor and the slurry bubble-column reactor. The active phase in FTS is metallic cobalt and the conventional type of catalyst precursors contain an oxide phase that has to go through activation under hydrogen at temperatures exceeding 250 ^{o}C. The use of such catalysts in slurry-phase reactors requires *ex situ* reduction and passivation of the catalyst before it is loaded into the slurry reactor, in order to prevent thermal damage and decomposition of the liquid medium in the slurry.

An alternative route to the metallic cobalt is via the carbide. This involves a carburization step under a CO-rich atmosphere followed by decomposition of the carbide to form the metal. This occurs under hydrogen at relatively low temperatures (<250 ^{o}C) and can be done in the slurry liquid medium. However, the effect of the CO pre-treatment on the catalyst performance remains under debate. This study focuses on the pre-treatment in CO and subsequent decomposition of the carbide to form an active catalyst. The process is studied both with advanced characterization techniques and by investigating the catalytic activity in the Fischer-Tropsch synthesis.

Publications and presentations in 2016:

1. Eleni Patanou, Nikolaos E. Tsakoumis, Rune Myrstad, Edd Anders Blekkan, *The impact of sequential H_2-CO-H_2 activation treatment on the structure and performance of cobalt based catalysts for the Fischer-Tropsch synthesis* (2016) *Submitted*.
2. Eleni Patanou, Nikolaos E. Tsakoumis, Rune Myrstad, Edd Anders Blekkan, *The effect of CO pre-treatment on a Co/Re /γ-Al2O3 catalyst for Fischer-Tropsch synthesis*, NGCS11 - 11th Natural Gas Conversion Symposium, June 5-9, Tromsø, Norway.

Financial support:
NTNU Department of Chemical Engineering, SINTEF Materials and Chemistry.

Strategy to Rapidly Screen Heterogeneous Transition Metal Catalysts: Microkinetic Analysis of Steam Methane Reforming from Combined DFT Calculations and UBI-QEP Method

Ph.D. Candidate: Yalan Wang
Supervisor: Prof. De Chen

Computational catalyst screening based on microkinetic modeling among heterogeneous transition metal catalysts for quickly predicting the activity and selectivity trends has gained much attention in recent years. Density functional theory (DFT) calculation is the most popular method to estimate the input parameter and generate the scaling relationship as well as descriptors of microkinetic models with high accuracy. While the DFT calculations will

spend much time and be computationally expensive. The unity bond index-quadratic exponential potential (UBI-QEP) method, formerly known as the BOC-MP (Bond-order-conservation Morse-potential) method, is also a commonly used approach for estimation of adsorption heats by theoretical calculations. However, low accuracy is a main problem for UBI-QEP method. In the present study, UBI-QEP theory is modified according to DFT estimated adsorption heats to increase the accuracy. Brønsted-Evans-Polanyi (BEP) relationships are applied to obtain activation energies based on DFT calculations. We use steam methane reforming (SMR) as a test reaction for UBI-QEP estimated microkinetic modeling, with C- and O-metal binding energy as descriptors of the model. SMR is a process to convert natural gas into synthesis gas or hydrogen, which can be further for producing higher value chemicals. Moreover, SMR is potentially important in emerging hydrogen economy due to as a source of hydrogen. Although various studies have been applied in the research of SMR, the exact reaction mechanism is still under debate. In this work, several possible mechanisms are combined together to build the model by using CatMAP (Catalysis Microkinetic Analysis Package), a software package to describe catalytic trends with descriptor-based microkinetic mapping.

DFT calculations are performed by using the Vienna Ab-initio Simulation Package (VASP) code. The calculation is proceed firstly on the fcc(111) surface of Nickel, then applied in other metal surfaces, such as Rh, Pt, Pd, Co and so on. The adsorption heats and activation energies for the elementary steps of SMR are estimated by DFT calculations, UBI-QEP method and BEP relationships, respectively. In the previous work, UBI-QEP method has been modified which can satisfactorily fit the DFT estimated adsorption energies and experimental catalytic trends among several transition metal surfaces. The predicted catalytic trend is: Rh > Ni ~ Co > Pt ~ Pd > Cu > Fe, consistent with experimental results. The modified UBI-QEP method combined with BEP relationship reduces radically the computational expenses, but keeps the accuracy compared to DFT calculation, therefore could be applied in the first step of catalyst design for rapid screening high activity catalysts for heterogeneous reactions, with C-, H- and O-metal binding energy as three sole descriptors.

Publications and presentations in 2016:

1. Y. Wang**,** Y. Qi, Y. Zhu, D. Chen, Mechanism research of light olefin formation in Fischer-Tropsch synthesis over cobalt catalysts by combination of DFT calculations and microkinetic analysis. Poster presentation. 11th Natural Gas Conversion Symposium, Tromsø, Norway. June 5-9, 2016.
2. Y. Wang, Y. Qi, Y. Zhu, D. Chen, Mechanistic research of light olefin formation in Fischer-Tropsch synthesis over cobalt catalysts by combination of DFT calculations and UBI-QEP method. Poster presentation. 16th International Congress on Catalysis, Beijing, China. July 3-8, 2016.

Integrated H_2BioOil process for efficient biofuel production

Ph.D. Candidate: Isaac Yeboah
Supervisor: Prof. De Chen
Co-supervisor: Dr. Kumar Ranjan Rout

Innovational research and development for transport fuel generation technologies from renewable (lignocellulose) resources have attracted global concern due to the associated climate change and CO_2 emissions from Fossil sources. There are several pathway to produce fuel from lignocellulose biomass such as gasification, hydrolysis and pyrolysis. Pyrolysis of lignocellulose, cheaply exploitable biomass source, gives low quality bio-oil due to its high acid value (TAN), oxygen content and energy density (16-19 MJ/kg). Therefore, to meet the transportation fuel standard a catalytic upgrading is required.

In this project, an in-situ generated H_2 gas and lignocellulose feedstock will be fed to the fast-hydropyrolysis (FHP) reactor. The FHP reactor is integrated with a catalytic reactor, having carbon coupling and hydrodeoxygenation (HDO) catalyst, to improve the carbon density and fuel properties of the pyrolysis-vapors respectively. Thus, ketonization, aldol condensation, esterification and hydrodeoxygenation (HDO) reactions will be optimized on cheaply and rationally designed Cu, Ni, and Zn based bimetallic catalyst supported on Nitrogen doped CNT or TiO_2, in tandem with Au/SiO_2 and Zeolite. Thus, embodies, applied catalyst design to activate these reactions in the single reactor with a dual bed. In that, a systematic studies in a continuous flow high pressure reactor will be executed to understand the effects of process conditions (temperature, pressure, feed flow-rate, biomass type etc.) on FHP as well as an integrated downstream upgrading reactor.

Comprehensive catalyst characterization techniques such as TPD, XPS, STEM, FTIR, BET, and XRD etc. are employed on the realistically designed catalyst while the product identification and quantification (conversion, yield and selectivity) are done in a multi-purpose installed GC-FID, GC-MS (NIST11 library), and HPLC-MS.

Financial support:
The project is funded by the Research Council of Norway under the ENERGIX research program

In situ and *ex situ* characterisation of iron based catalysts during CO_2-rich Fischer-Tropsch Synthesis

Postdoctoral Fellow: Dr. Diego Alexander Pena Zapata
Supervisor: Prof. Magnus Rønning

Fischer-Tropsch Synthesis (FTS) for synthetic hydrocarbon production from coal, natural gas and biomass-derived syngas (X to liquids processes) are well-established industrial processes being the subject of considerable fundamental and applied research. The syngas (H_2/CO) feed originated from biomass can be rich in CO_2, therefore operating FTS without syngas purification may give a simpler process at lower cost. Iron catalysts are attractive for BTL applications, in view of their capacity to manage non-stoichiometric syngas, to work at

higher temperatures and their lower cost, although they have lower FTS activity compared to Co. Optimization of catalyst performance is a very important issue. Activation of the iron oxide catalyst precursors in H_2, CO, H_2/CO seems to be crucial with the aim to increase catalyst stability and activity. Another important topic for improving Fischer-Tropsch catalyst technology is to improve catalyst deactivation.

The project aims to study the catalytic behaviour of FTS catalysts activated in different gas atmosphere (CO, H_2, and syngas (H_2/CO=2)). Several catalyst systems are tested; supported iron, unsupported iron (bulk), Cu-promoted and un-promoted catalysts. Catalyst activity and stability are evaluated in a fixed bed reactor rig. A wide range of *ex situ* and *in situ* characterisation techniques are used in order to reveal changes in active iron phases during pre-treatment (activation) and FT performance, as well as understanding the causes for deactivation. Catalyst are characterised before and after reaction by several *ex situ* techniques such as: X-ray Diffraction (XRD), Scanning Transmission Electron Microscopy (STEM), Thermal Gravimetric Analysis - Mass Spectroscopy (TGA-MS), Temperature Programmed Hydrogenation (TPH) and Gas Chromatography - Mass Spectroscopy (GC-MS). *In situ* FT-IR (at NTNU) and X-ray Diffraction (XRD) and X-ray Absorption Spectroscopy (XAS) are performed at the Swiss Norwegian beamlines (SNBL) at ESRF, France. The results lead to better catalyst activation protocols, active carbide phase identification and a deeper understanding of catalyst deactivation mechanisms.

Financial support:
The work is funded by the European FP7 project FASTCARD (FAST industrialization by CAtalysts Research and Development), Grant agreement no: 604277.

Presentation in 2016:

1. D. Peña, L. Saue Jensen, A. Cognigni, W.van Beek, M. Rønning, *The effect of copper loading on carbide phase formation in iron based catalysts during CO2-rich Fischer-Tropsch synthesis: In-situ X-ray absorption spectroscopy/high-resolution X-ray powder diffraction studies,* 11th Natural Gas Conversion Symposium, June 2016, Tromsø, Norway

2. M. Rønning, *Fischer-Tropsch synthesis catalysts: Strategies to enhance the sensitivity of in situ characterization techniques,* Invited lecture: 251st ACS National Meeting, March 13.-17. 2016, San Diego, USA

Supercapacitor with high gravimetric capacitance, volumetric capacitance and good rate capability

Ph.D. Candidate: Xuehang Wang
Supervisor: Prof. De Chen
Co-supervisor: Dr. Edel Sheridan

Specific energy of a supercapacitor (SC) in ionic liquid (IL) electrolyte is larger than that in an aqueous or an organic electrolyte due to the large voltage window of the IL electrolyte. However, the specific capacitance and the specific energy in IL suffer a serious reduction as the rate of charge/discharge increases for high power applications, which limits the wide-scale application of the high-energy SCs in IL. Any rising of the capacitance, both gravimetrically

and volumetrically, at high charge/discharge rate in the IL electrolyte results in a great improvement of specific energy for high power application.

We design and synthesize a densely-knitted macroporous framework with hierarchical porous structure. Notably, works until now focused on improving either gravimetric capacitance (sacrifice volumetric capacitance) or volumetric capacitance (sacrifice gravimetric capacitance). However, our material showed a comprehensive outstanding performance in IL: high gravimetric and volumetric capacitance with good rate capability. Based on our knowledge, the SC using the optimized material (RC600A850) in this work exhibits higher energy (162Wh/kg and 86 Wh/L), both volumetrically and gravimetrically, than the literature reported energy at low-power region. Due to the good rate capability, a full-packaged SC with the material can store/release energy comparable to a Ni-metal hydride battery (40-60 Wh/kg) gravimetrically and one order of magnitude higher than a commercial carbon-based SC volumetrically, within 1 min.

Presentation and poster in 2016:

1. Oral presentation. 'Favorable Ion Packing in Porous Carbon for High Gravimetric Capacitance Supercapacitors'. 229th ECS meeting, San Diego, US, 2016.
2. Trial lecture. 'Recent progress in electrochemical production and conversion of hydrogen'. Sep, 2016.

Publications in 2015

1. Xuehang Wang, Haitao Zhou, Fengliu Lou, Yahao Li, Marthe Emelie Melandsø Buan, Xuezhi Duan, John Charles Walmsley, Edel Sheridan and De Chen. Boosted supercapacitive energy with high rate capability in ionic liquid on a densely-knitted carbon framework with hierarchical pore structure. ChemSusChem, 2016, DOI: 10.1002/cssc.201600779.
2. Xuehang Wang, Yahao Li, Marthe Emelie Melandsø Buan, De Chen. Enhancing capacitance of supercapacitor with both organic electrolyte and ionic liquid electrolyte on a biomass-derived carbon. RSC Advances, 2017, DOI: 10.1039/c7ra01630a.
3. Haitao Zhou, Xuehang Wang, Edel Sheridan, Hongquan Gao, Juan Du, Jianhong Yang, and De Chen. Boosting the energy density of 3D dual-manganese oxides-based Li-ion supercabattery by controlled mass ratio and charge injection. Journal of Electrochemical Society**.** 2016, 163(13): A2618-A2622.

Financial support:
The project is funded by NTNU and the Norwegian Research Council.

Catalytic Conversion of Lignocellulosic Biomass to Chemicals and Fuels

Ph.D. Candidate: Cornelis van der Wijst
Supervisor: Prof. De Chen
Co-supervisor: Prof. Edd A. Blekkan

Today, transportation fuels and chemicals are mainly produced from fossil carbon sources. Due to the declining reserves and environmental effects, a transition to renewable carbon sources, like biomass, is important. Lignocellulosic biomass, such as trees, is the most

abundant biomass and one of the most promising renewable carbon sources. It is however very complex and relatively resistant to chemical transformation, making it difficult to exploit. In recent years interesting results have been published on using hot compressed water as a reaction medium for the conversion of lignocellulosic biomass. The hot compressed water has an excellent ability to facilitate the disintegration of lignocellulose, making it accessible for catalytic conversion into a variety of smaller oxygenates.

Our research is focused on developing the hot compressed water process and catalytic systems to selectively convert lignocellulosic biomass into a variety of chemicals and fuels. We have investigated ZnO-coated CNT as a composite support for Ni and Cu catalyst. The composite support gives basic character and a large surface area. The large surface area provides the basis for a large metal-ZnO interphase and enhances the formation of alloys. The alloys proved to be highly active in the direct conversion of cellulose to vicinal diols, e.g. ethylene glycol and 1,2-propylene glycol, through combining retro-aldol condensation reaction and hydrogenation reactions. The same catalyst and reaction conditions were simultaneously used to convert the lignin fraction to its monomeric phenolic compounds, enabling this process to directly convert raw lignocellulosic biomass in one single step.

Presentation:
C. van der Wijst, X. Duan, I. Skeie Liland, J. C. Walmsley, J. Zhu, A. Wang, T. Zhang, and D. Chen, Tuning the Selectivity of the Diols Produced From Cellulose on Nickel-Zinc alloys. Poster. 16th International Congress on Catalysis, Beijing, China, 2016.

Aqueous electrochemical CO_2 reduction on CuZnOCNT catalysts

Ph. D. Candidate: Ida Hjorth
Supervisor: Prof. De Chen

If CO_2 could be recycled by an artificial photosynthesis process, fuels could be sustainably produced and carbon neutral. CO_2 can be reduced electrochemically to small organic molecules, with photo-voltaic systems as the energy source. Unfortunately, there is no good catalyst for CO_2 reduction, so the process has not yet reached industrial feasibility. Copper is an interesting transition metal for catalyzing the reaction, on which a variety of hydrocarbons, alcohols and organic acids, as well as CO, are produced. However, the energy efficiency, conversion and selectivity is low. Therefore, much effort is needed to improve the catalysts.

By increasing the surface area, the catalytic efficiency can be improved. This can be achieved by supporting catalyst nanoparticles on carbon nanomaterials. These nanomaterials may have high electrical conductivity and surface area, and is therefore interesting as supports for electro-catalysts. By combining copper with other metals, the activity can also be changed.

In this project, Cu-Zn-CNT based catalysts have been tested for electrochemical reduction of CO_2 in water. Hydrogen, methane and CO products are quantified. In general, a syngas composition suitable for the Fischer-Tropsch process is obtained.

Financial support: Strategic funding, Norwegian University of Technology and Science

SINTEF projects

Gasification and FT-Synthesis of Lignocellulosic Feedstocks (GAFT)

Project category: KPN-project in ENERGIX. Project responsible is SINTEF Energy Research
Staff: Research Scientist Rune Myrstad and Senior Scientist Bjørn Christian Enger: SINTEF

The overall objective of the GAFT project is to contribute to accelerated implementation of liquid biofuels production in Norway. Particular attention is paid to feedstock mixing and torrefaction of challenging biomass enabling entrained flow (EF) gasification, EF gasification technology development and medium scale Fischer-Tropsch synthesis (FTS) development based on synthetic gas from the EF gasifier.

SINTEF MK is responsible for the FTS work package. The major objective of the FTS work package is to demonstrate iron based medium to high temperature FT technology for the production of liquid biofuels. In the GAFT project, an iron based FT catalyst will be utilized in a medium to high temperature range for synthesis of biocrudes from the gasifier syngas.

Client: The Research Council of Norway and the project partners; Avinor, Silva Green Fuels, Viken Skog SA, EcoPro AS, CAMBI AS, Johnson Matthey and SP Energy Technology Center.

Hydrotreating

Staff: Research Scientist Håkon Bergem, Senior Engineer Camilla Otterlei, SINTEF.

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 TCMD

Refinery operations / Octane processes

Staff: Research scientist Hilde Bjørkan, Senior Engineer Camilla Otterlei 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 TCMD

Fischer Tropsch synthesis

Staff: Senior Scientist Bjørn Christian Enger, Senior Scientist John Walmsley, Research Scientist Rune Myrstad, Reserch Scientist Jia Yang, Research Scientist Øystein Dahl, Research Scientist Martin F. Sunding, Senior Scientist Julian Tochard, Senior Scientist Rune Lødeng, Research Manager Torbjørn Gjervan

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

Client: SABIC

FAST industrialisation by CAtalysts Research and Development (FASTCARD 2014 - 2017)

Project category: EU 7th FP (NMP) "Exploration, optimisation and control of nano-catalytic processes for energy applications"; SINTEF is project coordinator (Duncan Akporiaye)

Staff SINTEF (WP3, Hydrotreating, BTG lead): Senior Scientist Rune Lødeng (co-work package leader) and Hilde Bjørkan (Dept. Kinetics and Catalysis), John Walmsley and Ingeborg Helene Svenum (Dept. Materials physics).

Short Description

Liquefaction of biomass by fast pyrolysis leads to a bio-oil comprising oxygenated and reactive sugar-derived as well as lignin-derived products. Hydrotreatment of such feeds is attractive both for stabilization (storage) and chemical conversion (transportation fuels, or co-feed). Up to now, R&D has focused on full oxygen removal (HDO) which is energy (and hydrogen) demanding. A more attractive alternative is by mild treatment (conditioning/stabilisation) to partially deoxygenated products, with an oxygen content allowing co-processing in existing refineries. Alternative non-noble metal containing nano-scale catalysts are aimed at to efficiently hydrogenate such oils.

WP3 will develop new generation catalysts for two levels of hydrotreating, i.e. the bio-oil stabilization and the further upgrading by a more severe hydrodeoxygenation (SINTEF focus is study of intrinsic kinetic performance and advanced characterization, ZrO_2 supported molybdenum oxide and carbide based catalyst systems, phenol as model feed), with the objective to produce co-feed to existing FCC units while minimizing the level of treatment. Challenges are the robustness of catalyst performance, lowering the hydrogen consumption, reducing process severity (lower pressure and temperature, and higher space velocity), to improve durability, and increase selectivity in relation to oxygen removal.

Client: EU

Publications:

1. Daria Otyuskaya, Rune Lødeng, Joris W. Thybaut, Guy B. Marin, "*Microkinetics assisted analysis of hydrotreating selectivities in fast pyrolysis oil upgrading*", Presentation Europacat 2015 (FASTCARD publication)
2. Rune Lødeng, Presentation at KinCat group meeting 29. April 2016. "*The Fastcard project – Hydrotreating of phenolics*".
3. Rune Lødeng, Chanakya Ranga, Tapas Rajkowa, Vaios Alexiadis, Hilde Bjørkan, Svatopluk Chytil, Ingeborg-Helene Svenum, John Walmsley, Joris Thybaut, Presentation at Cascatbel workshop, "*Catalytic HDO of phenolics in the gas and liquid phase over supported MoO_3 and its pre-carburized analogues*", 18 – 20 May 2016, Porto Carras, Chalkidiki, Greece
4. Chanakya Ranga, Rune Lødeng, Joris W. Thybaut, Poster presentation Cascatbel workshop, "*Insights into the activity of supported Mo oxide and their (oxy)-carbide analogues in catalytic conversion of biomass derived oxygenates*"
5. Chanakya Ranga, Rune Lødeng, Joris W. Thybaut, Poster presentation NCCC (Dutch catalysis meeting), "*Gas Phase Anisole Hydrodeoxygenation over Supported Mo oxide and*
6. *carbide catalysts as an alternative to Mo sulfides*"
7. Daria Otyuskaya, Rune Lødeng, Joris W. Thybault, Guy B. Marin, "*Anisole hydrodeoxygenation over non-sulphided CoMo/γ-Al_2O_3: experimental investigation and kinetic model construction*", in submission
8. Rune Lødeng, Chanakya Ranga, Tapas Rajkowa, Vaios Alexiadis, Hilde Bjørkan, Svatopluk Chytil, Ingeborg-Helene Svenum, John Walmsley, Joris Thybaut, "*Hydrodeoxygenation of phenolics in liquid phase over supported MoO_3 and carburized analogues*", Submitted for Biomass Conversion and Biorefinery, 211216 (Invited paper after Cascatbel workshop in Greece, May 2016)
9. Chanakya Ranga, Rune Lødeng, Tapas Rajkhowa, Vaios I. Alexiadis, Hilde Bjørkan, Svatopluk Chytil, Ingeborg H. Svenum, John Walmsley, Joris W. Thybaut, "*Activity and stability of supported molybdenum oxide and carburized catalysts for anisole hydrodeoxygenation*", Submitted for ACS Catalysis (under revision, to be resubmitted 090217)

EmX 2025 – an R&D base for reduced exhaust emissions in the Norwegian marine transportation sector

Project Category: Researcher Project from the Research Council of Norway
Staff: Research Scientist Jia Yang and Senior Scientist Rune Lødeng

Distribution of liquefied natural gas (LNG) is developing in Norway as well as globally, and represents an option for efficient and more environmentally friendly marine propulsion. With LNG as fuel, it is critical that methane emissions (methane slip) are controlled to very low levels since methane is a greenhouse gas with 20 times the global warming potential of CO_2. The proposed project targets new knowledge and innovation for emissions abatement, more specifically nitrogen oxides (NOx) and methane (CH_4) in the marine sector. It is a collaboration between NTNU and SINTEF. NTNU is focused on selective catalytic reduction and SINTEF is focus on methane abatement for natural gas engine in marine sector. Success criteria are to obtain >90% methane conversion below 500 °C in excess of oxygen, presence of H_2O and CO_2, and possibly also potential poisons like NOx, NH_3, SOx and S (from fuel,

lubricant or added as odorant). Highly active and stable catalysts based on transition metal oxides are to be developed.

Client: The Research Council of Norway TRANSPORT2025 Program through Contract No. 246862 + An advisory board with industrial stakeholders (SINTEF Ocean, Gasnor, Bergen Engine AS, Yara) has been established.

Publications:

1. Yang, Jia; Lødeng, Rune; Venvik, Hilde Johnsen. *Co and Ni spinel catalysts for low temperature methane total oxidation.* 9th International Conference on Environmental Catalysis - ICEC 9; 2016-07-10 - 2016-07-13

Philosphiae Doctor (PhD) theses in 2016

Yanying Qi; *Mechanistic Insights into Cobalt-based Fischer-Tropsch Synthesis*. Doctorial thesis at NTNU, 2016: 106

Farbod Dadgar; *Direct synthesis of dimethyl ether in microstructured reactors; The interactions between methanol synthesis and methanol dehydration*. Doctorial thesis at NTNU, 2016: 179

Xuehang Wang; *Porous carbon prepared by chemical activation for high-energy supercapacitors in ionic liquid electrolyte*. Doctorial thesis at NTNU, 2016: 264

Disputas Yanying Qi 25.04.16. From left: Prof. De Chen, Prof. Zhixin Yu, UiS, Assoc. Prof. Brian Grimnes, NTNU, Prof. Manos Mavrikakis, University of Wisconsin, USA, Prof. Em Anders Holmen.

Disputas Farbod Dadgar 20.06.16. From left: Prof. Em. Anders Holmen, Dr. Florian Huber, hte, Germany, Farbod Dadgar, Prof. Alessandra Beretta, University of Milan, Prof. Jens Petter Andreassen, NTNU, Prof. Hilde Venvik

Disputas Xuehang Wang 30.09.16. From left: Prof. Elzbieta Frackowiak. Poznan University, Poland, Assoc. Prof. Brian Grimes, NTNU, Xuehang Wang, Dr. Alejandro Oyarce Barnett, SINTEF, Dr. Edel Sheriden, SINTEF, Prof. De Chen.

Master (Diploma) Students in 2016

Tor Erik Sørensen; *Catalytic conversion of kerogen in enhanced oil production from shales*

Debashish Chowdhury; *Synthesis and characterization of tungsten carbide*

Wei Ge; *Multifuctional proppants for enhanced oil production from shales*

Marthe Meyer*; Catalytic conversion of kerogen in enhanced oil production form shales*

Ellinor Sofie Smith Wiker; *Reactor model for oxychlorination of ethylene in multi-turbular fixed bed ractors*

Shawn Christopher Apan; *Photocatalytic H2-production through photo-reforming of hydrocarbons*

Annemari Løberg Larsen; *Reduction of Cu-ZnO water-gas shift catalysts in presence of water*

Mads Alexander Lid; *Efficient catalysts for achieving NO/NO_2 equilibrium*

Ole H. Bjørkedal; *Efficient catalysts for achieving NO/NO_2 equilibrium*

Benedicte Hovd; *Direct nonoxidative conversion of methane to C_2 hydrocarbons, aromatics and hydrogen*

Stine Lervold; *Establishing experimental and characterization methodology for analyzing the performance of silver catalysts for formalin production.*

Vegard Andreas Naustdal; *Characterization of Ag catalysts for formalin production*

Hanna Marie Storvik; *Catalysts for control of methane slip in marine machinery using platinum-based catalysts*

Helene Mørkkåsa Sandvik; *Catalysts for control of methane slip in marine machinery using palladium based catalyst*

David Kovacic; *Cellulose conversion by hybrid catalysts*

Thomas Neumayer; *Fischer-Tropsch synthesis catalysts for CO_2-rich syngas*

Marc Grauel; *Catalytic conversion of biomass in biphasic system*

Exchange Bachelor Students in 2016

Ruiyu Zhang; *Metal anticorrosion applications of electrochemical exfoliated graphene*

Yaki Qin; *Application of biomass derived carbon materials in waste oil recycling*

Exchange and Master Students in 2016

2015-2016 Master students at NTNU (from left to right): exchange student David Kovacic (Slovakia), Stine Lervold, Marthe Meyer, Ellinor Sofie Smith Wiker, Ole Bjørkedal, Vegard Andreas Naustdal, Mads Alexander Lid, Debashish Chowdhury, exchange PhD student Ting Cui (China). Photo: Estelle Vanhaecke, NTNU

Group meetings with seminars

Spring 2016

Location: K5-201

Schedule	Time	Presenter	Topic
Feb.5	14:00	Ljubisa Gavrilovic	*Influence of potassium species on cobalt based Fischer-Tropsch catalyst using aerosol deposition technique*
Feb.19	14:00	Estelle Vanhaecke	*The Solid Acid Fuel Cell Stack into APU system and The Cool Flame enabled EGR – from laboratory work to industrial applications*
Mars 4	14:00	Qingjun Chen	*Novel catalysts design on natural gas purification, conversion to syngas and further to liquids*
April 1	14:00	Anders Holmen	*Fischer-Tropsch Synthesis – the Effect of Water*
April 15	14:00	Endre Fenes Daham Gunawardana	*Quantitatively defining promotor influence on catalytic activity and stability in ethylene oxychlorination* *Understanding Catalytic Phenomena Responsible for Metal Dusting*
April 25	14:00	Yanying Qi	*PhD defence*
April 29	14:00	Rune Lødeng	*FASTCARD EU project – Hydrotreating of phenolics*
May 13	13:00	Diego Pena	*In-situ studies over iron-copper alumina supported catalysts during Fischer-Tropsch Synthesis*
May 27	14:00	Shirley Leland	*Towards active and stable Ni based bimetallic catalysts for steam methane reforming*
June 17	13:15	Prof. Xiulian Pan, Dalian Institute of Chemical Physics, Chinese Academy of Sciences	Seminar on Catalysis for Clean Fuels *Selectivity control in catalytic conversion of syngas*

Autumn 2016

Location: K5-428/429

Schedule	Time	Presenter	Topic
September 2	14:00	Opening of the new facilities.	
September 7	09:30	Prof. Krijn de Jong	Nanoscale effects in heterogeneous catalysis
September16	14:00	Isaac Yeboah	Highly selective renewable fuel from 1-propanol
September 30		Xuehang Wang	Disputas
October 14	14:00	Mari Helene Farstad	Water adsorption on TiO_x thin films on Au(111)
October 28	14:00	Maria Victoria Gil Matellanes	H_2 production by sorption enhanced steam reforming of biomass-derived compounds
November 11	14:00	Xavier Auvray	Microwave-assisted synthesis of Pt/Al_2O_3 catalyst
November 25	14:00	Yalan Wang	Strategy to Rapidly Screen Heterogeneous Transition Metal Catalysts: Microkinetic Analysis of Steam Methane Reforming from Combined DFT Calculations and UBI-QEP Method
December 9	14:00	Hilde J. Venvik	Centre for Industrial Catalysis Science and Innovation (iCSI – SFI)

Courses given by Group Members

TKP4110 Chemical Reaction Engineering

Coordinator: Professor Jens-Petter Andreassen

Lecturers: Professor De Chen,
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:
Basic 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, 2nd edition, 2013, and articles and handouts.

Exam: Written

TKP4155 Reaction Kinetics and Catalysis

Responsible: Professor Magnus Rønning
Lecturers: Professor Magnus Rønning

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: Professor Jens-Petter Andreassen
Lecturers: Assoc. prof. Estelle Vanhaecke, Dr. Sulalit Bandyopadhyay
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.

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
TKP4580 - Catalysis and Petrochemistry, Specialization Project 15 SP
TKP4581 - 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: Engineer Karin W. Dragsten, Professor Hilde J. Venvik

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

Course description:
The course is for 5th year students and new Ph.D. students, and is held 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 Hilde Venvik

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 2017.
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 (Hilde Venvik in 2016)

Credits: 7.5 SP

Course description:
The course is given every second year, next time in fall term 2018.
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 2018
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

Publications in 2016

1. Bokach, D.; Ten H., Sander; Muthuswamy, N.; Buan, M. E. M.; Rønning, M., **Nitrogen-doped carbon nanofiber catalyst for ORR in PEM fuel cell stack: Performance, durability and market application aspects**, *International Journal of Hydrogen Energy*, 2016, 41, 17616-17630

2. Buan, M. E. M.; Muthuswamy, N.; Walmsley, J.; Chen, D.; Rønning, M., **Nitrogen-doped carbon nanofibers on expanded graphite as oxygen reduction electrocatalysts**, *Carbon*, 2016, 101, 191-202

3. Dadgar, F.; Myrstad, R.; Pfeifer, P.; Holmen, A.; Venvik, Hilde J., **Direct dimethyl ether synthesis from synthesis gas: The influence of methanol dehydration on methanol synthesis reaction**, *Catalysis Today* 2016, 270, 76-84

4. den Otter, J. H.; Yoshida, H.; Ledesma, C.; Chen, D.; de Jong, K. P., **On the Superior Activity and Selectivity of PtCo/Nb_2o_5 Fischer Tropsch Catalysts,** *Journal of Catalysis*, 2016, *340*, 270-275.

5. Duan, X. Z.; Ji, J.; Yan, X. D.; Qian, G.; Chen, D.; Zhou, X. G., **Understanding Co-Mo Catalyzed Ammonia Decomposition: Influence of Calcination Atmosphere and Identification of Active Phase**, *ChemCatChem*, 2016, 8, 938-945

6. Duan, X. Z.; Wang, D.; Qian, G.; Walmsley, J. C.; Holmen, A.; Chen, D.; Zhou, X. G., **Fabrication of K-Promoted Iron/Carbon Nanotubes Composite Catalysts for the Fischer-Tropsch Synthesis of Lower Olefins,** *Journal of Energy Chemistry*, 2016, 25, 311-317

7. Esteban-Díez, G.; Gil, M. V.; Pevida, C.; Chen, D.; Rubiera, F., **Effect of Operating Conditions on the Sorption Enhanced Steam Reforming of Blends of Acetic Acid and Acetone as Bio-Oil Model Compounds,** *Applied Energy*, 2016, 177, 579-590

8. Feng, X.; Chen, D.; Zhou, X. G., **Thermal Stability of TPA Template and Size-Dependent Selectivity of Uncalcined Ts-1 Supported Au Catalyst for Propene Epoxidation with H_2 and O_2**, *RSC Advances*, 2016, 6, 44050-44056

9. Feng, X.; Liu, Y.; Li, Y.; Yang, C.; Zhang, Z.; Duan, X.; Zhou, X.; Chen, D., **Au/Ts-1 Catalyst for Propene Epoxidation with H_2/O_2: A Novel Strategy to Enhance Stability by Tuning Charging Sequence**, *AIChE Journal*, 2016

10. Fernandes, V. R. P.; Van der Bossche, M.; Knudsen, J.; Farstad, M. H.; Gustafson, J.; Venvik, H. J.; Grönbeck, H.; Borg, A., **Reversed Hysteresis during CO Oxidation over $Pd_{75}Ag_{25}$(100)**, *ACS Catalysis*, 2016, 6, 4154-4161

11. Gil, M. V.; Fermoso, J.; Pevida, C.; Chen, D.; Rubiera, F., **Production of Fuel-Cell Grade H-2 by Sorption Enhanced Steam Reforming of Acetic Acid as a Model Compound of Biomass-Derived Bio-Oil**, *Applied Catalysis B: Environmental*, 2016, 184, 64-76

12. Huang, X.; Li, H.; Xiao, W. D.; Chen, D., **Insight into the Side Reactions in Methanol-to-Olefin Process over HZSM-5: A Kinetic Study**, *Chemical Engineering Journal*, 2016, 299, 263-275

13. Ledesma Rodriguez, C.; Yang, J.; Blekkan, E. A.; Holmen, A.; Chen, D., **Carbon number dependence of reaction mechanism and kinetics in CO hydrogenation on a Co-based catalyst**, *ACS Catalysis* 2016, 6, 6674-6686

14. Lei, J. Q.; Dong, H.; Duan, X. Z.; Chen, W. Y.; Qian, G.; Chen, D.; Zhou, X. G., **Insights into Activated Carbon-Supported Platinum Catalysts for Base-Free Oxidation of Glycerol**, *Industrial & Engineering Chemistry Research*, 2016, 55, 420-427

15. Lou, Fengliu; Buan, Marthe Emelie Melandsø; Muthuswamy, Navaneethan; Walmsley, John; Rønning, Magnus; Chen, De, **One-step electrochemical synthesis of tunable nitrogen-doped graphene**, *Journal of Materials Chemistry A*, 2016, 4, 1233-1243

16. Mahmoodinia, M.; Astrand, P. O.; Chen, D., **Influence of Carbon Support on Electronic Structure and Catalytic Activity of Pt Catalysts: Binding to the Co Molecule**, *Journal of Physical Chemistry C*, 2016, 120, 12452-12462

17. Phan, X. K.; Walmsley, J. C.; Bakhtiary Davijany, H.; Myrstad, R.; Pfeifer, P.; Venvik, H. J.; Holmen, A.**, Pd/CeO_2 catalysts as powder in a fixed-bed reactor and as coating in a stacked foil microreactor for the methanol synthesis**, *Catalysis Today* 2016, 273, 25-33

18. Romar, H.; Lillebø A. H.; Tynjälä P.; Hu T.; Holmen A.; Blekkan E. A.; Lassi U., **H_2-TPR, XPS and TEM Study of the Reduction of Ru and Re promoted Co/γ-Al_2O_3, Co/TiO_2 and Co/SiC Catalysts**, *Journal of Materials Science Research*, 2016, 5, 39-49

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30. Yang, J.; Frøseth, V.; Chen, D.; Holmen, A., **Particle size effect for cobalt Fischer-Tropsch catalysts based on in situ CO chemisorption**, *Surface Science* 2016, 648, 67-73

31. Zhang, J.; Sui, Z. J.; Zhu, Y. A.; Chen, D.; Zhou, X. G.; Yuan, W. K., **Composition of the Green Oil in Hydrogenation of Acetylene over a Commercial Pd-Ag/Al_2O_3 Catalyst**, *Chemical Engineering & Technology*, 2016, 39, 865-873

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Presentations in 2016

1. De Chen, **A New Insight into Reaction Mechanism of Fischer-Tropsch synthesis on Cobalt catalysts: A Combined Study of DFT and SSITKA**, 11th International congress of catalysis, July 3-8, 2016, Beijing, China.

2. De Chen, **Ni Based Steam Reforming Catalysts: From Molecular Understanding to Catalyst Design**, NGCS11 - 11th Natural Gas Conversion Symposium, June 5-9, Tromsø, Norway

3. De Chen, **Synthesis and applications of carbon based multifunctional catalysts for biomass conversion**. Symposium on carbon for catalysis (Carbocat), June 12-15, Strasbourg, France

4. De Chen **Methane steam reforming on Ni based bimetallic catalysts,** Symposium on nano and interfacial catalysis, July 7-13, Dalian, China.M. Rønning, **Fischer-Tropsch synthesis catalysts: Strategies to enhance the sensitivity of in situ characterization techniques**, Invited lecture: 251st ACS National Meeting, March 13-17, San Diego, USA

5. M. Rønning, **Nitrogen-doped carbon nanofibres as alternative catalysts for the oxygen reduction reaction in PEM fuel cells**, Invited lecture: SUNCAT seminar, March 21, Stanford University, USA

6. Rytter, E.; Holmen, A.; **Deactivation and regeneration of commercial type Fischer-Tropsch Co catalysts**. Invited lecture. 251th ACS National Meeting & Exposition; March 13-17, San Diego, USA

7. Holmen, A.; Rytter, E., **Selectivity of C_{5+} in Co-based Fischer-Tropsch synthesis**. Invited lecture. 251th ACS National Meeting & Exposition; March 13-17, San Diego, USA

8. Mahmoodinia, Mehdi; Åstrand, Per-Olof; Chen, De, **CO Activation on Edge Functionalized Graphene-based Pt Clusters: Electronic and Catalytic Properties**, Girona Seminar 2016: "Predictive Catalysis: Transition-Metal Reactivity by Design", April 17-20, Girona, Spain

9. Chen, Qingjun; Svenum, Ingeborg-Helene; Qi, Yanying; Gavrilovic, Ljubisa; Chen, De; Holmen, Anders; Blekkan, Edd Anders, **Potassium adsorption behaviors on hcp cobalt: A density functional theory calculation**, NGCS11 - 11th Natural Gas Conversion Symposium, June 5-9, Tromsø, Norway

10. Dam, Anh Hoang; Wang, Hongmin; Liland, Shirley Elisabeth; Holmen, Anders; Chen, De, **The methane adsorption activation energy dependency on different three-hollow sites**, NGCS11 - 11th Natural Gas Conversion Symposium, June 5-9, Tromsø, Norway

11. Fenes, Endre; Rout, Kumar Ranjan; Baidoo, Martina Francisca; Fuglerud, Terje; Chen, De, **Quantitatively defining promotor influence on catalytic activity and stability in ethylene oxychlorination**, NGCS11 - 11th Natural Gas Conversion Symposium, June 5-9, Tromsø, Norway

12. Gavrilovic, Ljubisa; Blekkan, Edd Anders; Venvik, Hilde Johnsen; Holmen, Anders; Brandin, Jan, **Influence of potassium species on Co based Fischer-Tropsch catalyst,** NGCS11 - 11th Natural Gas Conversion Symposium, June 5-9, Tromsø, Norway

13. Guo, Xiaoyang; Panditha Vidana, Daham S G; Vanhaecke, Estelle Marie M.; Hwang, Jihye; Walmsley, John Charles; Chen, De; Venvik, Hilde Johnsen, **Material degradation by metal dusting corrosion on instrumentation used in natural gas conversion technologies**, NGCS 11 - 11th Natural Gas Conversion Symposium, June 5-9, Tromsø, Norway

14. Ledesma C., Yang J., Blekkan E. A., A. Holmen, D. Chen: **The Use of Multicomponent SSITKA as a Tool to Study the Reaction Mechanism in CO Hydrogenation over Cobalt Catalysts.** Oral presentation, NGCS11 - 11th Natural Gas Conversion Symposium, June 5-9, Tromsø, Norway.

15. Patanou, Eleni; Tsakoumis, Nikolaos; Myrstad, Rune; Blekkan, Edd Anders, **The effect of CO pre-treatment on a Co/Re /γ-Al2O3 catalyst for Fischer-Tropsch synthesis**, NGCS11 - 11th Natural Gas Conversion Symposium, June 5-9, Tromsø, Norway

16. Qi, Yanying; Yang, Jia; Aaserud, Christian; Holmen, Anders; Chen, De, **Mechanistic insights into olefin selectivity on cobalt-catalyzed Fischer-Tropsch synthesis**, NGCS11 - 11th Natural Gas Conversion Symposium, June 5-9, Tromsø, Norway

17. Wang, Yalan; Qi, Yanying; Zhu, Yi-An; Chen, De, Mechanism research of light olefin formation in **Fischer-Tropsch synthesis over cobalt catalyst by combination of DFT calculations and microkinetic analysis**, NGCS11 - 11th Natural Gas Conversion Symposium, June 5-9, Tromsø, Norway

18. Yang, Jia; Eiras, Sara Boullosa; Myrstad, Rune; Pfeifer, Peter; Venvik, Hilde Johnsen; Holmen, Anders**, Fischer-Tropsch Synthesis on Co-Based Catalysts in a Microchannel Reactor: Effect of Temperature and Pressure on Selectivity and Stability**, NGCS11 - 11th Natural Gas Conversion Symposium, June 5-9, Tromsø, Norway

19. Østbye Pedersen, Eirik; Svenum, Ingeborg-Helene; Blekkan, Edd Anders, **Co-Mn catalysts for Fischer-Tropsch production of light olefins**, NGCS11 - 11th Natural Gas Conversion Symposium, June 5-9, Tromsø, Norway

20. Zhu, Yi-An; Chen, De, **Descriptor-based microkinetic analysis of propane dehydrogenation**, 24th International Symposium on Chemical Reaction Engineering, June 12-15, Minneapolis Minnesota, U.S.A

21. Strømsheim, Marie Døvre; Knudsen, Jan; Guo, Xiaoyang; Sørvik, Linn Cecilie; Fernandes, Vasco Rafael; Venvik, Hilde Johnsen; Borg, Anne. **Near ambient pressure**

XPS investigation of CO oxidation over Pd3Au(100). 17th Nordic Symposium on Catalysis (NSC17), June 14-16, Lund, Sweden

22. Chen, Qingjun; Svenum, Ingeborg-Helene; Qi, Yanying; Gavrilovic, Ljubisa; Chen, De; Holmen, Anders; Blekkan, Edd Anders, **Potassium adsorption behavior and its influence on the CO adsorption and activation on hcp cobalt in Fischer-Tropsch synthesis**, 16th ICC, July 3-8, Beijing, China

23. Liland, Shirley Elisabeth; Yousaf, Bilal; Rout, Kumar Ranjan; Wang, Yalan; Chen, De, **Unprecedented Active and Stable Ni-Co Bimetallic Catalyst for Steam Methane Reforming**, 16th ICC, July 3-8, Beijing, China

24. Qi, Yanying; Yang, Jia; Aaserud, Christian; Holmen, Anders; Chen, De, **New insights to the effect of water on selectivity in cobalt catalyzed Fischer-Tropsch synthesis**, 16th ICC, July 3-8, Beijing, China

25. Wang, Yalan; Qi, Yanying; Zhu, Yi-An; Chen, De, **Mechanistic research of light olefin formation in Fischer-Tropsch synthesis over cobalt catalyst by combination of DFT calculations and UBI-QEP method**, 16th ICC, July 3-8, Beijing, China

26. Yang, Jia; Lødeng, Rune; Venvik, Hilde Johnsen, **Co and Ni spinel catalysts for low temperature methane total oxidation**, 9th International Conference on Environmental Catalysis - ICEC 9, July 10-13, Newcastle, Australia

27. Farstad, Mari Helene; Strømsheim, Marie Døvre; Knudsen, Jan; Guo, Xiaoyang; Gavrilovic, Ljubisa; Fernandes, Vasco Rafael P; Borg, Anne; Venvik, Hilde Johnsen, **CO oxidation over Pd-based alloys**, CMD26, September 4-9, Groningen, The Netherlands

28. Farstad, Mari Helene; Strømsheim, Marie Døvre; Svenum, Ingeborg-Helene; Borg, Anne; Venvik, Hilde Johnsen, **The effect of K impurities on Co(11-20) with respect to Fisher-Tropsh catalysis**, CMD26, September 4-9, Groningen, The Netherlands

29. Zhu, Yi-An; Chen, De, **Rational Catalyst Design for Propane Dehydrogenation**, 8th International Conference on Molecular Simulations and Informatics Technology Application. September 24-26, Dalian, China

30. M. E. M. Buan, N. Muthuswamy, A. Cognigni, J. C. Walmsley, D. Chen, and M. Rønning, **Nitrogen-Doped Carbon Nanofibers for the Oxygen Reduction: The Role of Iron As Growth Catalyst**, ECS PRiME 2016, October 2-7, Honolulu, USA

31. Mahmoodinia, Mehdi; Chen, De; Åstrand, Per-Olof, **Platinum clusters with a carbon support material as catalysts: ReaxFF simulations and DFT calculations**, Magical Mystery Tour of Electron Correlation, October 24-26, Oslo, Norway

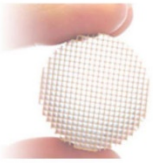
32. Volynkin, A.; Rønning, M.; Blekkan, E.A.; **Carbon-supported platinum catalysts: the role of carbon supports in hydrogenation/dehydrogenation model reactions.** CarboCat, June 12-15, Strasbourg, France

33. Strømsheim, Marie Døvre; Svenum, Ingeborg-Helene; Mari Helene; Farstad; Borg, Anne; Venvik, Hilde Johnsen, **CO single crystal surfaces as Fischer.Tropschmodel systems: STM investigations of alkali metal on Co single crystal surface**. NGCS11 - 11th Natural Gas Conversion Symposium, June 5-9, Tromsø, Norway

Popular science articles

Venvik, Hilde Johnsen; Lødeng, Rune. **Feil om katalysator.** Dagens næringsliv. September 2016.

Seminars 2016



iCSI

sfi Centre for Research-based Innovation

NTNU – Trondheim Norwegian University of Science and Technology

Seminar on Catalysis for Clean Fuels

Catalysis group, Department of Chemical Engineering, NTNU

KV-201, June 3, 2016

13:00-13:35: **The Mechanistic similarities for methane oxidation and reforming on transition metal and alloy clusters**
Prof. Ya-Huei (Cathy) Chin, Department of Chemical Engineering and Applied Chemistry, Toronto University, Canada.

13:35-14:10: **New catalyst and new process in C1 chemistry**
Prof. Noritatsu Tsubaki, Department of Applied Chemistry, University of Toyama, Japan.

14: 10-14:45: **Ethanolysis of kraft lignin over Mo-based catalysts**
Prof. Yongdan Li, Department of Chemical Engineering, Tianjin University, China

14:45-15:20: **Hydrodeoxygenation of bio-oil model molecules. Reaction mechanism and catalyst deactivation**
Prof. Fábio Bellot Noronha, Instituto National de Technologia, Rio de Janeiro, Brazil

KinCat

Catalysis Group – SINTEF – NTNU

Seminar Heterogeneous Catalysis

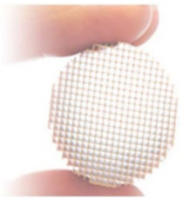
Monday, June 13, 2016

Professor Em. Hans Schulz

Karlsruhe Institute of Technology (KIT), Karlsruhe, Germany

Selforganizaton in Fischer-Tropsch synthesis with iron- and cobalt catalysts

The seminar will be given at 13:00 in K5-201, (Lunsjrom 2 etasje, Kjemiblokk V).



iCSI

Centre for Research-based Innovation

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Norwegian University of Science and Technology

KinCat
Catalysis Group – SINTEF – NTNU

Seminar on Catalysis for Clean Fuels

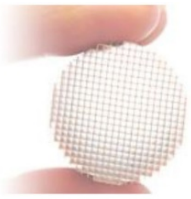
Catalysis group, Department of Chemical Engineering, NTNU

The seminar will take place at the Group Meeting on

Friday June 17, 2016 at 13:15 in KV-201

Professor Xulian Pan, Dalian Institute of Chemical Physics,
Chinese Academy of Sciences, China

Selectivity control in catalytic conversion of syngas



iCSI

Centre for Research-based Innovation

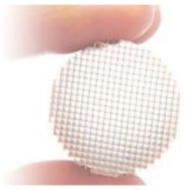
NTNU – Trondheim Norwegian University of Science and Technology

iCSI Kick off Seminar November 23-24 2016

Wednesday November 23 2016

Rådssalen, Main Building, NTNU

11.30-12.00	**Registration**
12.00-12.30	**Welcome opening** Professor Johan E. Hustad, Pro-rector Innovations, NTNU Dr. Odd-Arne Lorentsen, iCSI Board Chairman, YARA International Professor Hilde Venvik, iCSI Director, NTNU
12.30-13.30	**Lunch**
13.30-14.30	**IIAs Presentations by IIA leaders and Industrial Seniors** IIA 1 *21st century Ammonia Oxidation and Nitric Acid technology development* IIA 2 *New NOx abatement technologies for the marine market and state-of-the-art SCR catalysis* IIA 3 *Frontier formalin technology development* IIA 4 *PVC Value Chain: World class energy and raw material efficiency for the production of Chlorine and Vinylchloride Monomer (VCM)* IIA 5 *The next step in direct activation of lower alkanes*
14.30-15.00	**Coffee Break**
15.00-15.45	**The iCSI Scientific Advisory Committee presents** ***Title of the presentation*** by Professor Alessandra Beretta, Politechnico di Milano
16.30-19.30	**Team building activity**
20.00-22.00	**iCSI Dinner** ***Banksalen Restaurant*** ***Kongens Gate 4, 7010 Trondheim***



iCSI

Centre for Research-based Innovation

NTNU – Trondheim
Norwegian University of Science and Technology

Thursday November 24 2016

Konferansesenteret i SpareBank 1 SMN
Søndre gate 4, 7011 Trondheim

9.00-10.30	**Research presentations – 20 min + questions** IIA 5 *Dimitrios Pappas and Michael Dyballa, UiO/Haldor Topsøe* IIA 4 *Kumar Ranjan Rout, SINTEF/NTNU* IIA 1 *Reducing platinum losses during ammonia combustion,* SINTEF/UiO/Yara/KA Rasmussen
10.30-11.45	**Posters Session –** Snacks / Coffee will be served
11.45-12.30	**Panel discussion Industrial Committee / SAC**
12:30 -13.00	**Closing session** iCSI Industrial Poster prize iCSI SAC poster prize Closing remarks
13.00-14.00	**Lunch**

NGCS 11 Tromsø 2016

The 11th Natural Gas Conversion Symposium

Natural Gas Conversion Board

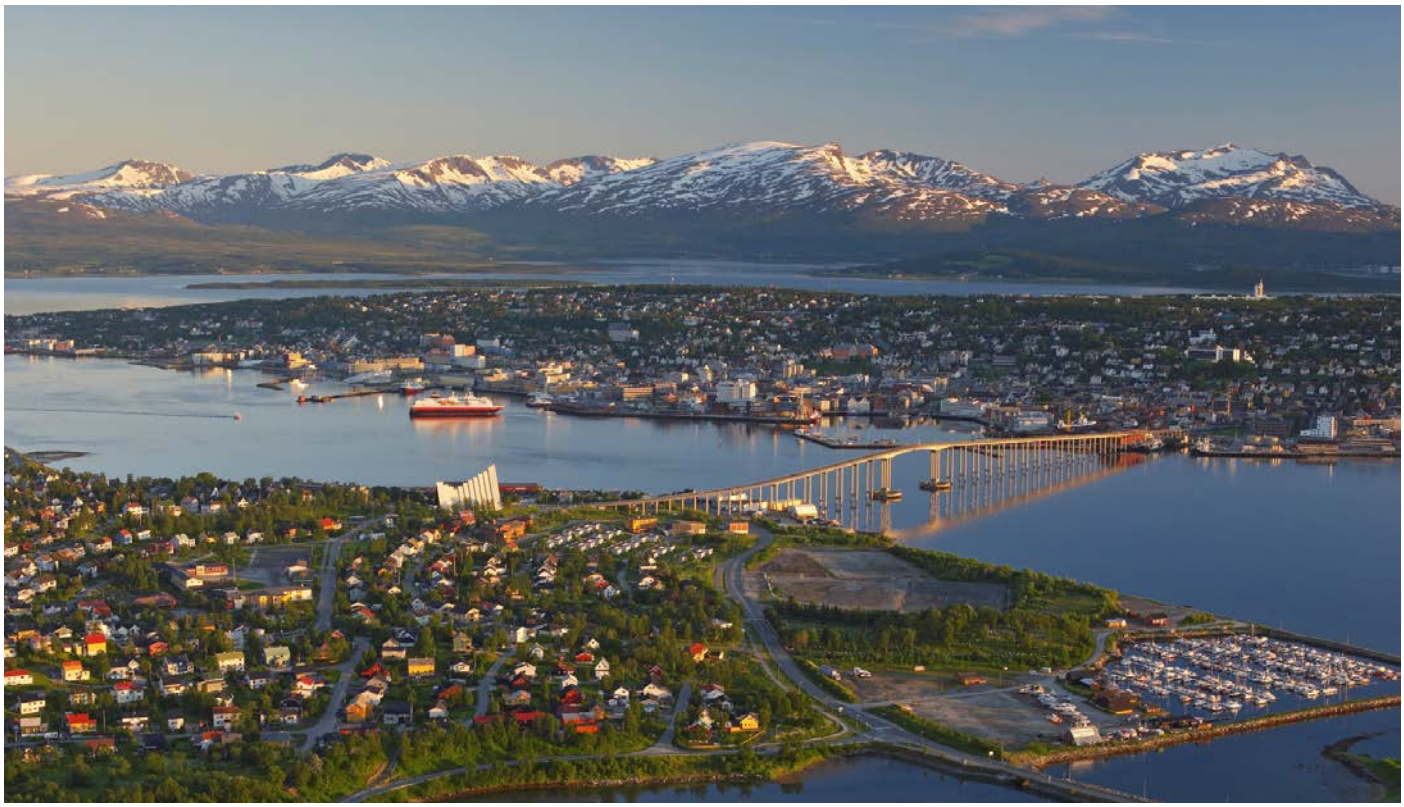


Photo: Bård Løken Destinasjon Tromsø

5 – 9 June 2016

Clarion Hotel *the Edge*

Tromsø, Norway

ExxonMobil

The Research Council of Norway

HALDOR TOPSØE

Production of Synthesis Gas
Synthesis Gas to Fuels and Chemicals
Direct Conversion of Methane
Conversion of Light Paraffins
Natural Gas in Energy Conversion
Techno-Economic Aspects

NTNU

Welcome to the Gateway to the Arctic!

Dear Natural Gas Conversion Colleagues!

It is a great pleasure to welcome you all to the 11th Natural Gas Conversion Symposium in Tromsø - 69°40′58″N! This edition of the premier NGC symposia series brings delegates close to abundant sources of natural gas, only partially discovered to date, in the Arctic. These resources are located far from the market, and their exploration, production and transport are associated with considerable challenges related to the conditions and climate.

Tromsø may be the northernmost place you will ever visit - the city's location and ice-free harbor are central to its long history as the gateway to the Arctic for hunters, fishermen and explorers. More recently, Tromsø has served as a gateway for those exploring Arctic oil and gas resources and home to the world's most northerly university. Tromsø has also become a tourist hotspot for experiencing the midnight sun or the northern lights. Well above the Arctic Circle, the sun does not set between May 21 and July 21. We hope that our social program enables you to connect with colleagues from around the world while enjoying the stunning scenery.

The ever changing resource and market situation around natural gas has brought about impressive changes, but also insecurity, in the natural gas based industries and markets. In addition, we must endeavour to show how natural gas conversion can contribute to a solution with respect to reduceing emissions and climate change. The only answer to this is research and development, with industry and academia working hand in hand. It is therefore appropriate that we can gather here together to explore natural gas conversion science and technology day and night!

We would like to express our appreciation to all that have contributed to NGCS 11. The Research Council of Norway, ExxonMobil, Haldor Topsoe, and Shell are providing generous support, demonstrating a consistent commitment to natural gas conversion R&D. The Local Organizing Committee has involved representatives from the main academic and industrial groups involved in natural gas conversion in Norway, i.e. the University of Oslo, SINTEF, Statoil, and Inovyn, in addition to the Norwegian University of Science and Technology (NTNU). Envoy Limited, TromsøEvent, Clarion, and VisitTromsø have all contributed to providing the best possible arrangements, venue and experience. The LOC has worked closely with the Natural Gas Conversion Board and its International Scientific Advisory Board, but also relied on contributions from a large number of external reviewers to produce a high-quality program and an inspiring environment for talented young researchers aspiring to a career in natural gas conversion!

With best wishes for an exciting and productive week in Tromsø,

Hilde Venvik

Anders Holmen

The Award for Excellence in Natural Gas Conversion

Professor Xinhe Bao
State Key Laboratory of Catalysis
Dalian Institute of Chemical Physics
Chinese Academy of Sciences

Professor Xinhe Bao has been chosen as the recipient of the 2016 Award for Excellence in Natural Gas Conversion. The Award is presented every three years during the International Natural Gas Conversion Symposium to recognize enduring and significant contributions to science and technology for conversion of natural gas to valuable products. The previous award recipients are Krijn de Jong (2013), Anders Holmen (2010), David Trimm (2007), Enrique Iglesia (2004), Lanny Schmidt (2001), Jens Rostrup-Nielsen (1998), and Jack Lunsford (1993).

Professor Bao is recognized for his contributions to the fundamental understanding of the chemistry and engineering of gas conversion. His ability to combine theory, model catalysts, and technical catalysis in a very original manner has led to a number of breakthrough developments with both scientific and industrial impact. As specific contributions to the field of natural gas conversion three topics are highlighted. Firstly, the direct conversion of methane to aromatics using bifunctional Mo/ZSM-5 catalysts has been studied extensively by Professor Bao with important new structure-performance relationships that have enabled higher aromatic yields. Secondly, CO hydrogenation to fuels and chemicals has been investigated with special reference to the role of confinement of nanoparticles in catalysis. Thirdly, direct conversion of methane to lower olefins has been realized for the first time using a catalyst with isolated iron sites, with interest in this finding noted from both the scientific community and industry.

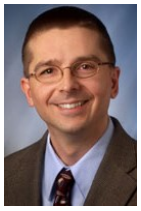
Professor Bao has been a long-standing leader in research programs on natural gas conversion related research in China. He is a member of the Chinese Academy of Sciences, the Academy of Sciences for the Developing world and a fellow of the Royal Society of Chemistry. He acts as chair and board member of international scientific conferences and was the chair of the 7th Natural Gas Conversion Symposium in Dalian. He serves on the editorial boards of a wide range of journals and book series relevant to natural gas conversion.

NGCS11 Plenary Lecturers

Jim Rekoske, Vice President & Chief Technology Officer, UOP

Jim Rekoske has global responsibility for general management of the research and development function at Honeywell's UOP, a leading developer and licensor of technologies for the oil, gas and petrochemical industry. Over nearly two decades with UOP, he has held positions of increasing responsibility in areas ranging from research and development, marketing, customer service and sales support, and technology strategy. He earned bachelor's and master's degrees in chemical engineering at the University of Wisconsin, a doctorate in chemical engineering from the University of Delaware, and an MBA degree from the University of Chicago's Booth School of Business.

Rekoske is the (co-)inventor to more than 30 U.S. patents, and the author of more than 20 peer-reviewed scientific articles. He was awarded the 2010 Herman Pines Award from the Chicago Catalysis Club in recognition of his numerous technical breakthroughs in catalysis.



Gary Jacobs, Principal Research Engineer Clean Fuels & Chemicals University of Kentucky Center for Applied Energy Research

Dr. Jacobs's research is focused on heterogeneous catalysis of syngas conversion for the production of ultra-clean fuels and chemicals, with an aim to link catalyst performance parameters (activity, selectivity, and stability) with electronic and geometric structure. His research relies heavily on the application of synchrotron techniques to develop insights at the atomic scale.

He received a B.S. in chemical engineering from University of Texas and a Ph.D. in chemical engineering from University of Oklahoma. He then joined the Clean Fuels & Chemicals research group of Prof. Burtron H. Davis at the University of Kentucky's Center for Applied Energy Research. The group has strong relationships with industry as well as state, federal, and international agencies. Jacobs has co-authored over 185 refereed publications and received, with Davis, four Elsevier top-50 most-cited-author awards for articles on Fischer-Tropsch synthesis and fuel processor catalysts for fuel cells.

Unni Olsbye, Professor, Chemistry Department University of Oslo

Professor Olsbye's field of expertise is heterogeneously catalysed processes, with an emphasis on structure-composition-function correlations and mechanistic studies on microporous catalysts (zeolites, MOFs), in parallel with activity related to reactions promoted by supported metal catalysts. Processes studied include methanol to hydrocarbons (olefins and gasoline), methane reforming and partial oxidation to syngas, light alkane dehydrogenation, methyl halide conversion, ethene oxychlorination and CO_2 conversion.

She graduated as a Chemical Engineer from the Norwegian University of Science and Technology (NTNU) and proceeded to work with Elf Aquitaine on a project which earned her a Ph.D. degree in chemistry at the University of Oslo (UiO). From 2007 – 2015 she was Managing Director of the inGAP (Innovative Natural Gas Processes and Products) National Excellence Centre. Olsbye has authored more than 100 scientific papers, holds several patents, and is an elected member of the Norwegian Academy of Science and Letters and the Norwegian Academy of Technical Sciences.

Local Organizing Committee (LOC)

Professor Hilde J. Venvik, Dept. of Chemical Engineering,
Norwegian University of Science and Technology (NTNU)

Professor Em. Anders Holmen, Dept. of Chemical Engineering,
Norwegian University of Science and Technology (NTNU)

Professor De Chen, Dept. of Chemical Engineering,
Norwegian University of Science and Technology (NTNU)

Erling Rytter, Special Advisor/Professor SINTEF/NTNU (prev Statoil)

Professor Unni Olsbye, Department of Chemistry, University of Oslo

Duncan Akporiaye, Vice President Research, SINTEF Materials and Chemistry

Steinar Kvisle, Director of Technology and Production Support, INOVYN

Tronn Hansen, Special Advisor, Research Council of Norway

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Dr. José Santiesteban *
ExxonMobil R&E, United States

Mr. Robert Saxton *
Chevron, United States

Prof. Reinhard Schomäcker
Technische Universität Berlin, Germany

Dr. Wataru Ueda
Science Univ. of Tokyo in Yamaguchi, Japan

From	To	SUNDAY JUNE 5	MONDAY JUNE 6	TUESDAY JUNE 7	WEDNESDAY JUNE 8	THURSDAY JUNE 9
08:00	08:30		**Registration**			
08:30	09:00		**Clarion Hotel the Edge**			
09:00	08:30		Plenary 1 Rekoske	Plenary 2 Jacobs	Plenary 3 Bao	Plenary 4 Olsbye
08:30	10:00		**Margarinfabrikken, Clarion the Edge**	**Margarinfabrikken, Clarion the Edge**	**Margarinfabrikken, Clarion the Edge**	**Margarinfabrikken, Clarion the Edge**
10:00	**10:30**		**Coffee break**	**Coffee break**	**Coffee break**	**Coffee break**
10:30	10:50		Parallell sessions.	Parallell sessions.	Parallell sessions.	Parallell sessions.
10:50	11:10		M1 M2 M3	M1 M2 M3	M1 M2 M3	M1 M2 M3
11:10	11:30		Topic 1 Topic 2 Topic 3	Topic 1 Topic 2 Topic 3	Topic 1 Topic 2 Topic 3	Topic 5 Topic 2 Topic 1-6
11:30	11:50					
11:50	12:10					
12:10	12:30					Closing ceremony
12:30	**13:00**		**Lunch**	**Lunch**	**Lunch**	
13:00	**13:30**		**Clarion Hotel the Edge**	**Clarion Hotel the Edge**	**Clarion Hotel the Edge**	**Lunch**
13:30	13:50		Parallell sessions.	Parallell sessions.	Parallell sessions.	**Clarion Hotel the Edge**
13:50	14:10		M1 M2 M3	M1 M2 M3	M1 M2 M3	
14:10	14:30		Topic 1 Topic 2 Topic 4	Topic 1 Topic 2 Topic 1-6	Topic 1 Topic 2 Topic 5	
14:30	14:50					
14:50	15:10			**Coffee break**		
15:10	15:40	**Registration 15:00**	**Coffee break**	Parallell sessions.	**Coffee break**	**Post-conference social activities**
15:40	16:00	**Clarion Hotel the Edge**	Parallell sessions.	M1 M2 M3	Parallell sessions.	
16:00	16:20		M1 M2 M3	Topic 1 Topic 2 Topic 6	M1 M2 M3	**Option 1 | Snøhvit LNG Site Visit**
16:20	16:40		Topic 1 Topic 2 Topic 5		Topic 5 Topic 2 Topic 4	**Option 2 | Boat / fishing excursion**
16:40	17:00					**Option 3 | Mountain hike w/NGCS chairs**
17:00	17:20			**Excursion &dinner**	**Poster session**	
17:20	18:00			**Departure hotel 17:00**	**Quality Hotel Saga**	**Booking required**
18:00	18:30		**Poster session**	**Sommarøy fishing village & island**	**With refreshments**	**- see NGCS11 website for details**
18:30	19:00		**Quality Hotel Saga**	**Return starts from approx. 22:00**		
19:00	19:30	**Welcome reception &**	**With refreshments** **NGCB**			
19:30	20:00	**opening ceremony**	**meeting**			
20:00	20:30	**Polaria Arctic Museum & Aquarium**	**the Egde**		**Conference Gala Dinner**	
20:30	21:00	**Drinks and light meal served**			**Clarion Hotel the Edge**	
21:00	21:30					
21:30	22:00					
22:00	22:30					
22:30	23:00					

Social Program

The social program developed by the NGCS 11 Local Organizing Committee provides delegates and those accompanying them with numerous opportunities to experience the best of Tromsø, Norway, and life north of the Arctic Circle, while providing time to build and maintain international networks with colleagues from academia, science, and industry involved in natural gas conversion. The program includes three parts.

Part 1 | Symposium Social Program

Sunday, June 5 19:00 | Evening welcome reception and exhibition
Polaria Arctic Museum & Aquarium
Drinks and light meal served
Suggested attire: Business casual

Tuesday, June 7 17:00 | Evening excursion and dinner
Bus trip to Sommarøy fishing village, including visits to
the Skavberget rock carvings and Viking graves at Greipstad.
Drinks and dinner served
Suggested attire: Casual, including sweater and windproof jacket/coat

Wednesday, June 8 20:00 | Gala Dinner at Clarion Hotel the Edge
Margarinfabrikken Ballroom
Drinks and dinner served
Suggested attire: Business

Part 2 | A Taste of Local Art, Food, Culture and Nature

Optional short excursions and tours primarily intended for accompanying persons (spouse / partner), with a limited number of places available by pre-registration. Any remaining places offered onsite. See registration desk for program and cost.
Official Tromsø visitor's guide: visittromso.no

Part 3 | Post-Symposium Program open to all delegates by pre-registration.

Option 1 | Snøhvit LNG Site Visit June 9 -10
Statoil hosts a limited number of NGCS 11 delegates at the world's northernmost LNG plant, located on Melkøya island just outside Hammerfest. The Snøhvit ("Snow White") gasfield is located 143 km from shore and was developed using only subsea installations with the multiphase flow sent through a pipeline to the LNG installation, where CO_2 in the gas is separated and returned to an underground reservoir.

Option 2 | Boat / fishing excursion June 9, 15.00 - 21.00
Enjoy Tromsø and the spectacular scenery from offshore aboard the N/S Caroline Mathilde, a classic wooden boat built in 1939 that can travel by motor or sail. And maybe catch your own dinner! A small meal will be served (fish soup or similar). Please note!
Warm clothing must be brought as the eather feels colder

at sea. Water-/windproof jacket, sweater (wool or fleece) and boots or trainers as a minimum.

Option 3 | Mountain hike with symposium chairs! 9 June, 15.00 - late.
Register within June 8 at Conference desk. NOK 100 for transportation to starting point. The target for the trip will be adapted to the weather conditions, but we aim for a local peak of 800-1000 m. Hence, reasonable fitness level and good knees required, but no need for climbing equipment/experience.
Important! Everyone must wear good hiking shoes or trainers and bring their own food/ drink/snack in a backpack. In good weather, we may opt for midnight sun and sea view at the top.

Monday June 6 09:00 – 10:00 Plenary Lecture:

Dr. Jim Rekoske, Vice President & Chief Technology Officer UOP

Technoeconomic Impacts of Abundant Natural Gas Liquids on the Chemical Industry

Session Chairs

Steinar Kvisle, INOVYN

Hilde Venvik, Department of Chemical Engineering, NTNU

1000-1030	COFFEE BREAK		
	Topic 1 - Dry reforming **Session chairs:** Fabio Noronha, Nat. Inst. Techn., Brazil De Chen, NTNU, Norway	**Topic 2 - MTO and MTH** **Session chairs:** Olaf Hinrichsen, TU München, Germany Stian Svelle, Univ. Oslo, Norway	**Topic 3 - CH_4 to aromatics** **Session chairs:** Yongdan Li, Tianjin U., China Edd Blekkan, NTNU, Norway
1030-1050	1172 CH_4 Conversion to Synthesis Gas over Supported Well-defined Pt, Rh, and Ru Nanoparticles: Effect of Metal, Nanoparticle Size and Support *V.A. Kondratenko, Leibniz Katalyse, Rostock U., Germany.*	0994 Methanol to Propylene (MTP™): A proven technology for on-purpose propylene production (and how we got there…) *M. Rothaemel, Air Liquide, Frankfurt am Main, Germany*	1007 Non-oxidative catalytic conversion of CH_4 to benzene with continuous catalyst regeneration in a dual circulating fluidized bed reactor system at 1073 K *Z.-G. Zhang, AIST, Tsukuba, Japan*
1050-1110	1155 New routes for Syngas production – Dry Reforming at elevated pressure *A Behrens, Linde AG, Pullack, Germany*	1091 Conclusive evidence for two unimolecular pathways to zeolite-catalyzed de-alkylation of the heptamethylbenzenium cation *M. Mortén, U. Oslo, Norway*	1008 Coke accumulation and removal behaviors of Mo/HZSM-5 in the non-oxidative CH_4 dehydro-aromatization under periodic CH_4-H_2 switching operation mode *Y. Song, AIST, Tsukuba, Japan*
1110-1130	1153 Catalytic dry reforming of methane over Ni/β-Mo_2C catalysts *V. Teixeira da Silva, Universidade Federal do Rio de Janeiro, Brazil*	1175 Mechanistic Insight in the Methanol-to-Olefins Reaction over Small-Pore Zeolite Catalysts using Operando UV/Vis Spectroscopy *J. Goetze, U. Utrecht, The Netherlands*	1068 Acetylene, an intermediate for methane conversion to C_4 products *I.-T. Trotus, Max Planck Institut für Kohlenforschung, Mülheim, Germany*
1130-1150	1265 Handling of metal dusting at the Statoil Tjeldbergodden methanol plant *E. Edwin, Statoil Trondheim, Norway*	1227 Insights into Reaction Pathways in Methanol to Hydrocarbons using Synchrotron Infrared Microspectroscopy *R. Howe, U. Aberdeen, UK*	1204 Direct non-oxidative methane coupling over modified gallium oxide photocatalyst. *H. Yoshida, Kyoto U. Japan*
1150-1210	Keynote 1 (1214) Catalytic Consequences of Reactive Intermediates for Methane Dry Reforming Reactions on First Row Transition Metal and Alloy Clusters *Ya-Huei (Cathy) Chin,U. Toronto, Canada.*	1277 Mechanism of coke formation in the conversion of methanol to olefins over H-ZSM-5 *Y. Liu,TU München, Germany.*	1233 A Fluidized Bed Natural Gas to Aromatics Process *F. Wei, Tsinghua U. Beijing, China*
1210-1230		1296 High throughput testing of catalyst with different time scales of deactivation for MTH *A. Haas, hte GmbH, Heidelberg, Germany*	1294 Direct conversion of methane to aromatics in a catalytic membrane reactor *S. Hernández Morejudo, Coorstek Membrane Sciences, Oslo, Norway*
1230-1330	LUNCH Restaurant Clarion Hotel the Edge		

Monday June 6, Continued

	Topic 1- Steam reforming **Session chairs:** A. Monzón Bescos, U. Zaragoza, Spain Zhixin Yu, Univ. Stavanger	**Topic 2 – Alcohols, DME** **Session chairs:** Krijn de Jong, U. Utrecht Klaus-Joachim Jens,U. Coll. S.-E. Norw.	**Topic 4 - Dehydro C_2H_6** **Session chairs:** Wataru Ueda, Kanagawa U., Japan Steinar Kvisle, Inovyn, Norway
1330 1350	1183 Shell impregnation of steam reforming catalyst *C.V. Ovesen, Haldor Topsøe A/S, Lyngby, Denmark*	1018 CNTs-Ni-Mo-K hybrid catalysts with enhanced performance for synthesis of higher alcohols from syngas *X. L. Liang, Xiamen University, China*	1103 Simulation-aided effective design of a catalytic reactor for ethane oxidative dehydrogenation *E. Heracleous, International Hellenic U., Thessaloniki-Moudania, Greece*
1350- 1410	1339 Towards active and stable Ni based bimetallic catalysts for steam methane reforming *S.E. Liland, NTNU, Norway*	1059 Direct synthesis of dimethyl ether from mixture of carbon oxides over copper alumina catalysts prepared using the sol-gel method *Kaoru Takeishi, Shizuoka U., Japan*	1305 Temporal Analysis of Products (TAP) – an advanced tool for time-resolved kinetic characterization of industrially-relevant microporous materials *E. A. Redekop, U. Oslo, Norway*
1410- 1430	1249 Compact Inexpensive Reformers for Natural Gas *J. Carpenter, RTI International, Durham, US*	1263 Impact of the catalyst synthesis of bifunctional catalysts on syngas to DME formation *D. Wendt, Max-Planck Institut fur Kohlenforschung, Mülheim, Germany*	1176 Design and performance of alternative-type ZrO_2-based catalysts for non-oxidative dehydrogenation of light alkanes *T. Otroshchenko, Leibniz Katalyze, Rostock U, Germany*
1430- 1450	1262 Catalyst performance assessment for low temperature steam reforming of methane via comprehensive microkinetic modelling *P.N. Kechagiopoulos, U. Aberdeen, UK*	Keynote 2 (1061) Roles of ZnO in methanol and methanol-dimethyl ether-combi catalysts *Sebastian Kuld, Haldor Topsøe A/S, Lyngby, Denmark*	1245 Porous clay heterostructures with columns made of titania as supports of NiO for the oxidative dehydrogenation of ethane *J. M. Lopez Nieto, ITQ, Valencia, Spain*
1450- 1510	1020 Modeling Development for a Combined Methane Fixed Bed Reactor Reformer *M. Elbashir, Texas A&M U. at Qatar, Qatar.*		1016 Low temperature, selective oxidative upgrading of ethane to value-added products, over Fe- and Cu-ZSM-5 catalysts *R.D. Armstrong, Cardiff U, UK*
1510- 1540	COFFEE BREAK		

Monday June 6, Continued

	Topic 1- Partial oxidation **Session chairs:** Alessandra Beretta, P. Milano, Italy Bjørn Chr. Enger, SINTEF, Norway	**Topic 2 – Co FT charact.** **Session chairs:** Andrei Khodakov, Univ. Lille, France Magnus Rønning, NTNU, Norway	**Topic 5 – CO_2 to SNG** **Session chairs:** Fabio Ribeiro, Purdue University., US Hilde Venvik, NTNU, Norway
1540-1600	1302 CPO of C_1-C_8 hydrocarbons: Kinetic analysis, Raman surface characterization and adiabatic testing *G. Groppi, Politecnico di Milano, Italy*	1025 Mapping the structure and chemical composition of nanoparticles with wide size distributions: a Ferromagnetic Nuclear Resonance study of Cobalt based nanoparticles for producing synthetic fuel *C. Meny, IPCMS,U. Strasbourg, France*	Keynote 3 (1308) Development of methanation catalysts for the process chain Power to Gas *Anne-Cécile Roger, ICPEES, U Strasbourg, France*
1600-1620	1297 On the control of the properties of electrosynthesized Rh-based syngas production catalyst *P.H. Ho, U. Bologna, Italy*	1030 Hydrocarbon chemistry on cobalt: surface science investigations of the FT chain growth mechanism *C.J. Weststrate, Syngaschem BV, Eindhoven, The Netherlands*	
1620-1640	1235 Novel $NiAl_2O_4$-based catalysts supported on ceria and ceria-zirconia for partial oxidation of methane. *R. Lopez-Fonseca, U. Basque Country, Spain*	1173 New insights on the aggregates of cobalt nanoparticles by electron tomography and anomalous X-ray scattering *S. Humbert, IFPEN, Solaize, France*	1312 Catalytic conversion of CO_2 to Synthetic Natural Gas (SNG) on Ru-based catalysts *L. Falbo, Politecnico di Milano, Italy*
1640-1700	1253 Study of Perovskites $LaNi_{1-x}Co_xO_3$ Catalysts in the Partial Oxidation of Methane *S.T, Brandao, U. Federal da Bahia, Brazil*	1192 *In situ* monitoring of supported cobalt catalysts for FTS under realistic conditions; what have we learned *N. Tsakoumis, NTNU, Norway*	1198 Production of synthetic natural gas by CO_2 methanation: Synthesis and characterization of highly active catalysts *O. Hinrichsen, TU München, Germany*
1700-1720	1289 Role of oxygen activation in the production of syngas by catalytic partial oxidation of methane over dual $LaMnO_3$-Pd/YSZ beds *M. Richard, U. Poitiers, France*	1237 Co single crystal surfaces as FT model systems: STM investigations of alkali metal on Co single crystal surface *M.D. Strømsheim, NTNU, Norway*	1217 Highly active NiO/CeO_2 catalysts for Synthetic Natural Gas production by CO_2 methanation *E. Rombi, U. Cagliari, Monserrato, Italy*
1800-2000	POSTER SESSION w/refreshments Quality Hotel Saga		

Tuesday June 7 09:00 – 10:00, Plenary lecture:

Dr. Gary Jacobs Principal Research Engineer

Center for Applied Energy Research, University of Kentucky, USA

Fischer-Tropsch synthesis: use of hard and soft X-rays in the characterization of catalysts and contaminants

Session Chairs:

Gordon Kelly, Johnson Matthey Catalysts, UK,
Erling Rytter, NTNU/SINTEF (prev. Statoil)

1000-1030	COFFEE BREAK		
	Topic 1 – Deactivation **Session chairs:** Cathy Chin, U. Toronto, Canada Rune Lødeng, SINTEF, Norway	**Topic 2 – FT mechanisms** **Session chairs:** Michael Claeys, U. Cape Town, S-Africa Anders Holmen, NTNU, Norway	**Topic 3 – OCM , Direct CH_4** **Session chairs:** Dae-Hoon Lee, KIMM, Rep. of Korea Magnus Rønning, NTNU, Norway
1030-1050	1038 Dry reforming of methane on Ni-based pyrochlore catalysts: Understanding carbon deposition mechanism *J. Spivey, LSU, Baton Rouge, US*	0992 Effect of CO coverage on the product slate in FTS. *H. Oosterbeek, Shell Global Solutions, Amsterdam, The Netherlands*	1105 The chemical looping concept in oxidative coupling of methane on the $Na_2WO_4/Mn/SiO_2$ catalyst: challenges and opportunities for catalyst investigation without gas phase O_2 *V. Fleischer, TU Berlin, Germany*
1050-1110	1098 Understanding the Effects of Support Chemical Composition on the Origin and Reactivity of Carbon Formed During Dry Reforming of CH_4 over $Ni/Ce_{1-x}M_xO_{2-\delta}$ (M=Zr4+, Pr3+) via Transient Isotopic Techniques *A. Efstathiou, U. Cyprus Nicosia*	1154 Spontaneous formation of cobalt nano-islands and kinetic role of hydroxyl species during Fischer-Tropsch synthesis *M. Saeys, U. Ghent, Belgium*	1292 Evaluation of the combination of oxidative coupling of methane with COx hydrogenation to increase production of C_2+ hydrocarbons *M. Albrecht, Leibniz Katalyse, Rostock U., Germany*
1110-1130	1058 Improving the sintering resistance of Ni/Al_2O_3 steam reforming catalysts *F. Morales Cano, Haldor Topsøe A/S, Lyngby, Denmark*	1075 Fischer-Tropsch synthesis on cobalt catalyst: A combined transient kinetic and mechanistic study *W. Chen, U. Eindhoven, The Netherlands*	1003 Partial oxidation of methane in gas phase at very short residence time: influence of NO and NO_2 on the yield and selectivity of formaldehyde *V. Burkle-Vitzthum, CNRS-U Lorraine, Nancy, France*
1130-1150	1006 Industrial scale reforming of CO_2-rich gas. *P. Mortensen, Haldor Topsøe A/S, Lyngby, Denmark*	1125 Microkinetic model validation for the FTS based on transient experiments *J. Van Belleghem, U. Ghent, Belgium*	1236 C to H effective ratio as a descriptor for dehydroaromatization of methane with light oxygenates on Mo/HZSM-5 catalyst *D.-Y. Hong, Korea Research Institute Chemical Technol., Rep. of Korea*
1150-1210	Keynote 4 (1340) Ni based steam reforming catalysts: from molecular understanding to catalyst design *De Chen, Department of Chemical Engineering, Norwegian University of Science and Technology (NTNU), Norway*	1112 Kinetics of methane formation and 1-olefin hydrogenation in FTS over cobalt catalyst *D.B. Bukur, Texas A&M U at Qatar, Doha, Qatar.*	1144 Direct Conversion of CH_4 to Methanol on ZSM-5 from First-principles. *A. Arvidsson, Chalmers U., Sweden*
1210 1230		1328 Identification of deactivation mechanisms of supported nickel and cobalt catalysts for syngas conversion using transient kinetic methods *A Carvalho, U. Lille, France*	1079 Direct conversion of methane over NiO and MgO catalysts supported on SBA-15 *T. Kim, Chosun U. Gwangju, Republic of Korea.*
1230-1330	LUNCH		

Tuesday June 7, Continued

	Topic 1-Dry reforming **Session chairs:** Charlotte Ovesen, H. Topsøe, Denmark Estelle Vanhaecke, NTNU, Norway	**Topic 2 – FT Co catalysts** **Session chairs:** Dragomir Bukur, Texas A&M, Qatar Edd Blekkan, NTNU, Norway	**Gas Hydrates, new concepts** **Session chairs:** Holli Garrett, Clariant, USA Hilde Venvik, NTNU, Norway
1330 1350	1168 Catalytic methane steam reforming at low temperature over Pd/CeO_2 in an electric field *R. Manabe, Univ. Waseda, Japan*	1234 The effect of thermal treatments on the characteristics of supported Cobalt FT catalysts *G. Kelly, Johnson Matthey, Billingham UK.*	Keynote 5 Arctic gas hydrates as unconventional energy *Jürgen Mienert, Centre for Arctic Gas Hydrate, UiT- The Arctic University of Norway, Tromsø*
1350- 1410	1048 Dry reforming of CH_4 on different supported Co catalysts *A. Erdöhelyi U. Szeged, Hungary*	1304 SMSI effects in $CoRu/TiO_2$ catalysts and consequences on the catalytic performance for FTS *A Martinez, ITQ, Valencia, Spain.*	
1410- 1430	1288 Knowledge extraction for dry reforming of methane from past publications using data mining tools *R. Yildirim, Bogazici U. Istanbul, Turkey*	1100 CO hydrogenation on cobalt-based FT catalysts: chlorine poisoning reveals the nature of the most active sites. *A Paredes-Nunez, U. Lyon-CNRS, France*	1295 The Internal Combustion Engine as a Natural Gas Reformer: Operating Conditions Proposed by Numerical Optimization. *H. Gossler, KIT, Karlsruhe, Germany*
1430- 1450	1259 Chemical loop dry reforming of methane with Ni-Ceria based catalysts *A. Löfberg, U. Lille - CNRS, France*	1317 Fischer-Tropsch Synthesis: Poisoning Studies for Co and Fe catalysts *B. Davis, U. Kentucky, US*	1027 Preparation of $Co-Mn/TiO_2$ catalysts for C_2-C_4 olefins production *F. Shayegh, RIPI, Tehran, Iran*
1450- 1520	COFFEE BREAK		
	Topic 5 – Energy , H_2 **Session chairs:** Peter Pfeifer, KIT, Germany Maria Victoria Gil Matellanes, NTNU	**Topic 2 – FT light olefins** **Session chairs:** Sebastian Kuld, H. Topsøe, Denmark Selene H. Morejudo, Coorstek, Norway	**Topic 6 – Techno-Economic** **Session chairs:** Mikhail Sinev, Semenov Institute, Russia Tronn Hansen, Research Council of Norway
1520- 1540	1231Production of Hydrogen and Graphene by Methane Decomposition on Ni-Cu/Biomorphic Carbon Catalysts *A Monzón Bescos, U. Zaragoza, Spain*	1171 Size and Promoter Effects in Supported Iron Fischer-Tropsch Catalysts: Experiment and Theory *J. Xie, Utrecht University, the Netherlands*	1002 New potentialities for utilization of associated petroleum gases in power generation and chemicals production *V. Arutyunov, Semenov Institute of Chemical Physics, Moscow, Russia*
1540- 1600	1239 Photocatalytic steam reforming of methane over platinum-loaded lanthanum-doped sodium tantalate photocatalysts prepared by a flux method *A Yamamoto, Kyoto U. Japan*	1110 Catalytic synthesis of light olefins and alkanes over FeOx/Anodic Alumina Oxide/Aluminum cartridges *R. Lødeng, SINTEF, Norway*	Keynote 6 (1311) Techno-economic Analysis of Individual and Integrated Oxidative Coupling of Methane processes *H.R. Godini, Berlin TU, UniCat BASF, Berlin, Germany*
1600- 1620	1145 Chemical looping steam reforming with *in-situ* CO_2 capture over CaO-based sorbents and NiO-based oxygen transfer materials: Generation of high-purity H_2 in a single step *A Lemonidou, Aristotle U. Thessaloniki, Greece*	1258 Carbon Deposition in Iron Catalyzed Production of Lower Olefins from Synthesis Gas: Effect of Activation Conditions *A.C.J. Koeken, Dow, The Netherlands*	
1700- ...	**EXCURSION TO SOMMARØY DEPARTURE 17:00**		

Wednesday June 8 09:00 – 10:00, Award Lecture:

Professor Xinhe Bao,

Dalian Institute of Chemical Physics, Chinese Academy of Sciences, China

New horizons in C_1 chemistry

Session Chairs

Krijn de Jong, Utrecht University, The Netherlands

Anders Holmen, NTNU, Norway

1000-1030	COFFEE BREAK		
	Topic 1 - Biosyngas **Session Chairs** Victor Texeira, U. Federal Rio de J., Brazil Bjørnar Arstad, SINTEF, Norway	**Topic 2 - FT catalysis** **Session Chairs** Philip Gibson, Sasol, South-Africa Rune Myrstad, SINTEF, Norway	**Topic 3 – OCM, plasma** **Session Chairs** Claude Mirodatos, IRCELYON, France Unni Olsbye, Univ. Oslo, Norway
1030-1050	1132 Steam reforming of toluene, methane and mixtures over Pt/Al_2O_3 and $Pt/CeO_2/Al_2O_3$ catalysts *F. Noronha, National Institute of Tecnology, Rio de Janeiro, Brazil*	1182 Structure–Performance Relationships for Carbon Deposition in Iron Fischer-Tropsch Catalysts *J. Xie, U. Utrecht, The Netherlands*	Keynote 7 (1177) Effective Plasma Process for Methane Direct Conversion to Acetylene. *D.H. Lee, Korea Institute of Machinery and Materials, Daejeon, Republic of Korea*
1050-1110	1026 Catalytic reforming of biomass gasification tars with bi- and trimetallic catalysts optimized with organosilane precursorss *V. Claude, U. Liege, Belgium*	1280 Development of nitrogen-rich mesoporous carbon supported iron-based catalysts for highly efficient FT *N, Tsubaki, U Toyama, Toyama, Japan*	
1110-1130	1207 Syngas production by means of biogas oxy-CO_2 reforming using Pt and Rh catalysts *F. Bimbela, U Navarra, Pamplona, Spain*	1320 Process intensification and simplification as key element towards decentral fuel production *P. Pfeifer, KIT Karlsruhe, Germany*	1169 Dry reforming of methane by the combination of non-thermal plasma and catalysis *C. Batiot-Dupeyrat, U. Poitiers, France*
1130-1150	1149 Structured nanocomposite catalysts of biofuels reforming into syngas: design and performance. *V. Sadykov, Boreskov Institute of Catalysis, Novosibirsk, Russia*	1000 Commercial roll-out of a smaller scale GTL technology. *N. Hargreaves, Velocys, Milton Park, UK*	1136 Oxidative coupling of methane over polyoxometalate supported catalysts in an electric field at low T. *S. Ogo, Waseda U., Tokyo, Japan*
1150-1210	1260 A kinetic study of Catalytic Partial Oxidation and Steam Reforming of Acetic Acid over Rh-supported catalysts *A Beretta, Politecnico di Milano, Italy*	1313 Intensification of the FTS through an highly conductive structured packed-bed reactor: a pilot-scale *C. Visconti, Politecnico di Milano, Italy*	1264 RedOx Behaviour and Catalytic Performance of $NaWMn/SiO_2$ Mixed Oxide in OCM *M. Sinev, Semenov Institute of Chemical Physics, Moscow, Russia*
1210 1230	1299 Synthesis gas production from glycerol with low steam/carbon ratio. *M. Menéndez, U. Zaragoza, Spain*	1064 Hydrocracking under Fischer-Tropsch conditions: on the distinct reactivity of paraffin and α-olefin primary products N. *Duyckaerts, Max Planck Institut für Kohlenforschung, Mülheim, Germany*	1037 Way to Improve Performance of OCM with Catalysts of Different Properties *W. Liang, SABIC, Houston, US*
1230-1330	**LUNCH**		

Wednesday June 8, Continued

	Topic 1 – Steam ref., CPO **Session Chairs** James J Spivey, LSU, US Evgeniy Redekop, Univ. Oslo, Norway	**Topic 2 – FT catalysis** **Session Chairs** Heiko Oosterbeek, Shell, the Netherlands Erling Rytter, NTNU/SINTEF, Norway	**Topic 6 – NG processes** **Session Chairs** Hamid Reza Godini, TU Berlin, Germany Jannike Solsvik, NTNU, Norway
1330 1350	1151 Production of Hydrogen Enriched Syngas by Combined CO_2-Steam Reforming of Methane Over The Polymetallic Co-based Catalysts. *S. Itkulova, Sokolsky Institute, Almaty, Kazakhstan*	1088 Advances in Fischer-Tropsch technology at Shell *G.L. Bezemer, Shell Global Solutions, Amsterdam, The Netherlands*	990 Economically feasible small-scale GTL technology by INFRA Technology. Journey from laboratory to an industrial plant *V.Z. Mordkovich, INFRA Tech., Russia*
1350- 1410	1180 Steam Reforming of LPG over $Ni/CeZrO_2/Al_2O_3$ catalysts *F. Noronha, Instituto Nacional de Tecnologia. Rio de Janeiro, Brazil*	1256 Metal-support interactions in Co-Al_2O_3 model catalysts for FTS *A Petersen, U. Cape Town, South-Africa*	1303 Global solution for mercury removal in saturated wet gas streams: from rational material design to innovative process issues. *A Hugon, IFPEN, Solaize, France*
1410- 1430	1205 Co-Mn catalysts for Fischer-Tropsch production of light olefins E. Østbye Pedersen, NTNU, Norway	1341 *In-situ* thermal stability and reactivity investigation of Co-based nanostructures by environmental TEM *S. Moldovan, IPCMS, Strasbourg U, France*	1162 Synthesis and characterization of advanced nanomaterials for hydrogen sulfide removal in gas processing. *V. Vicentini, Clariant, Brazil*
1430- 1450	1228 Catalyst Development and Reactor Design for Catalytic Partial Oxidation of Natural Gas to Produce Synthesis Gas *S. Kado, Chiyoda Corporation, Japan*	Keynote 8 Stability of CO hydrogenation catalysts *M. Claeys, U. Cape Town, South Africa.*	1221Membrane-Integrated Systems for biogas separation *G. Barbieri, ITM-CNR, Rende, Italy*
1450- 1510	1167 Steam CO_2 Reforming of CH_4 over La_{1-x} Sr_xNiO_3 Perovskite Catalysts *G.H. Hong, KIST, Republic of Korea*		1319 Novel ionic liquid technology for mercury removal *H. Garrett, Clariant, Louisville, US*
1510- 1540	COFFEE BREAK		
	Topic 5 – SNG, combust., H_2 **Session chairs** Anne-Cécile Roger, U Strasbourg, France Jia Yang, SINTEF, Norway	**Topic 2 – FT Co catalysis** **Session chairs** Burtron Davis, U. Kentucky, US Nikos Tsakoumis, NTNU, Norway	**Topic 4 – Ethane , propane** **Session chairs** Randall Meyer, ExxonMobil, USA Anders Holmen, NTNU, Norway
1540- 1600	1174 Understanding Aging Processes during Bio-Syngas Methanation for Synthetic Natural Gas Production *C. Mirodatos, IRCELYON-CNRS-UCBL Lyon, France*	0993 Fischer-Tropsch catalyst deactivation in commercial operations *A P Steynberg, Velocys, Plain City, US*	1063 Molecular level insight of selective oxidation of ethane using a micropore of crystalline $Mo_{29}V_{11}O_{112}$ as a catalysis field *W. Ueda, U. Kanagawa, Yokohama, Japan*
1600- 1620	1031 Methane light-off simulation for catalytic converter application *N. Sadokhina, Chalmers U., Göteborg, Sweden*	1005 Effects of ordered mesoporous Co_3O_4 structures incorporated with irreducible metal oxides for an enhanced activity of FTS *J.W. Bae, U. Sungkyunkwan, Rep. of Korea*	1238 Influence of promotors in defining catalytic activity and stability quantitatively for oxychlorination process *E. Fenes, NTNU, Trondheim, Norway*
1620- 1640	1143 Low-Temperature Catalytic Combustion of Methane Studied by *In Situ* XAFS *J. Nilsson, Chalmers U., Sweden*	1071 Steric effects in the Fischer-Tropsch synthesis over cobalt nanoreactors *V. Ordomsky, U. Lille, France*	Keynote 9 (1247) Selective C-H Bond Activation by Supported Pt_1Zn_1 Nanoparticle Alloys during the Catalytic Dehydrogenation of Ethane *F. H. Ribeiro, Purdue U, West Lafayette, US*
1640- 1700	1318 Production of pure H_2 through CH_4 oxy-reforming process coupled with Pd-dense membrane reactor. *F. Basile, U. Bologna, Bologna, Italy*	1223 Hydrothermal resistance of alumina-supported FT catalysts: mechanism of the alumina transformation and identification of sensitive sites *J. Abi Aad, IFPEN-UPNC, France*	
1700- 1900	POSTER SESSION w/refreshments		
2000	**CONFERENCE DINNER**		

Thursday June 9 09:00 – 10:00, Plenary lecture:

Professor Unni Olsbye,

Department of Chemistry, University of Oslo, Norway

MTH revisited, status and prospects from fundamental studies

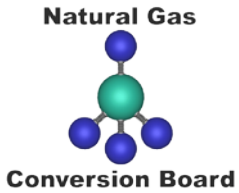
Session Chairs

Gabor Kiss, ExxonMobil

De Chen, NTNU, Norway

1000-1030	COFFEE BREAK		
	Topic 5 – SNG, combust., H_2 **Session chairs** Reinhard Schomäcker TU Berlin, Germany Ingeborg-H. Svenum, SINTEF, Norway	**Topic 2 – MTX, FTS** **Session chairs** Gary Jacobs, U. Kentucky, US Eleni Patanou, NTNU, Norway	**Topic 4 – Olefins, SSITKA** **Session chairs** Olaf Deutschmann, KIT, Germany Yanying Qi, NTNU, Norway
1030-1050	1067 First-principles microkinetic modeling of CH_4 oxidation over PdO(101) *M. Van den Bossche, Chalmers U, Göteborg, Sweden*	1023 Influence of post-synthetic treatments on unidirectional ZSM-22 zeolite catalyst: Towards improved clean gasoline catalytic process *P. del Campo, Univ. Oslo, Norway*	1250 Supported metal oxide catalysts for natural gas upgrading: Synergistic effect at sub-monolayer coverage to boost productivity toward olefins *Joseph Grant, UW Madison, US*
1050-1110	1187 Upgrade of substitute natural gas (SNG) via CO_2 hydrogenation – an *in situ* perspective *N. Fischer, U. Cape Town, South-Africa*	1141 Characterization and studies of Si and Brønsted site developments in SAPO-18 and SAPO-34 during and after hydrothermal treatment. *B.Arstad, SINTEF*	1099 Direct 1,3-butadiene production out of n-butane and butenes in a two-zone fluidized bed reactor with Mo based catalysts. *J. Rischard, KIT, Karlsruhe, Germany*
1110-1130	1191 Improve the Stability of Ni-$Ce_{0.8}$ $Sm_{0.2}$ O $_{1.9}$ as the anode of a CH_4 fuelled solid oxide fuel cell by Sn doping *Yongdan Li, Tianjin U. Tanjin, China*	1074 Highly active and stable Fischer-Tropsch catalysts obtained through unconventional Metal-Organic Framework mediated synthesis *F. Kapteijn, TU Delft, The Netherlands*	1322 Multi scale kinetics for the selective oxidation of propane to acrylic acid: Multi-route mechanism *C. Sprung, Fritz-Haber Institut, Germany*
1130-1150	1209 The effect of catalyst pellet size on nickel carbonyl-induced particle sintering under low temperature CO methanation. *J. Barrientos, KTH, Stockholm, Sweden*	*Keynote 10* (1092) Development of commercial type cobalt Fischer-Tropsch catalysts. *P. Gibson, Sasol Group Technology, Sasolburg, South Africa*	1307 Oligomerization of ethene with nickel containing beta zeolite at high pressure. *M. Kømurcu,. Oslo U., Norway*
1150-1210	1291 Catalytic Hydrogenation of Carbon Dioxide over Supported Nickel on Macro-/Mesoporous Titania-Alumina *S. Ernst, TU Kaiserslautern. Germany*		1332 The Use of Multicomponent SSITKA as a Tool to Study the Reaction Mechanism in CO hydrogenation over Cobalt Catalysts *Jia Yang, NTNU/SINTEF, Norway*
1220-1250	***CLOSING CEREMONY***		
1300-1410	LUNCH		

PosterSession:
http://ngcb.org/index.asp?sid=64



The triennial Natural Gas Conversion Symposium (NGCS) series began in 1987, with the aim of bringing together scientists and engineers from academia and industry working in the field of natural gas conversion. The NGCS is an independent, non-advocacy, non-commercial international event unconnected with any scientific, commercial, or government organization. The orderly continuation of the symposia series is overseen by a non-profit corporation - the Natural Gas Conversion Board - established for this purpose.

The Board's International Scientific Advisory Board (ISAB) is charged with assuring the technical excellence of the symposia and administering the Award for Excellence in Natural Gas Conversion, while its International Finance Committee (IFC) is responsible for encouraging corporate support for the symposia

See you at NGCS 12 in 2019!

Trial Lectures for the PhD degree

Edd Anders Blekkan: *Katalytisk hydrogenbehandling*. 18/12 1985.

Dag Schanke: *Katalytiske egenskaper til ikke-oksydiske keramer*. 1986.

Kjell Moljord: *Methods for controlling the content of aromatics in gasoline.*

Edvard Bergene: *Katalytisk rensing av eksosgasser*. 12/3 1990.

Rune Lødeng: *Technologies for formation of synthesis gas.* 1991

Trude Dypvik: *Syntesegass fra metan*. 30/1 1992

Ola Olsvik: *Catalytic membrane reactors*. 1993

Anne Hoff: *Production of i-butene*. 1993.

Stein Harald Skaare: *The Use of Transient Techniques in Kinetic Studies*. 10/12 1993.

Odd Arne Bariås: *Application of Rare Earth in Catalysis*. 2/12 1993.,

Geir Remo Fredriksen: *Catalytic combustion*. 17/12 1993.

Arne Grønvold: *Oxygenates as Fuel Components – Processes and Applications*. 9/9 1994.

Sturla Vada: *Spillover in catalysis*. 26/10 1994

Rune Prestvik: *Upgrading of light (C_2-C_4) alkanes by catalytic processes*. 1995

Anne-Mette Hilmen: *Catalysis by Solid Super Acids*. 8/10 1996

Karina Heitnes Hofstad: *Chemical nitrogen fixation*. 4/12 1996.

Håkon Bergem: *Preparation of Supported Metal Catalysts.* 16/4 1997.

Staale Førre Jensen: *Catalytic fixation of carbon dioxide*. 1998.

Mimmi Kjetså: *Methods for Controlling the Content of Aromatics in Gasoline*. 5/5 1998

De Chen: *Prevention of deactivation due to coke deposition. A multiscale approach*. 1998

Hans Petter Rebo: *Alkylation processes based on solid catalysts*. Mars 1999

Marit Senum A. Brownrigg: *In situ Production of Hydrogen for Fuel Cells in Cars*. 19/8 1999

Ketil Firing Hanssen: *The Role of Hydrogen in the Production of Hydrogen*. 15/12 1999

Magnus Rønning: *Photocatalysis*. 2/3 2000

Marcus Fathi: *Heterogenization of homogeneous catalysts*. 3/10 2000

Torbjørn Gjervan: *Recent advanced in direct conversion of methane*. 30/11 2000

Thomas Sperle: *Nanostructured Materials in Heterogeneous Catalysis*. 2001.

Lucie Bednarova: *Computational Catalysis.* 2002

Sten Viggo Lundbo: *Materials and processes for selective adsorption of* CO_2. 2002

Leiv Låte: *Catalysis in supercritical fluids*. 2002

Petr Steiner*: Transportation fuels and fuel components from biomass. Raw materials, production and performance*. 16/1 2002

Bozena Silberova; *Catalytic combustion*. 24/1 2003.

Christian Aaserud: *Catalytic Materials for Fuel Cell Applications*. 28/4 2003.

Kjetil Hauge: *Non-conventional routes to petrochemicals and fuels fromnatural gas.*2004

Thomas Løften*: Catalytic removal of nitrogen oxides under oxidizing conditions*. 16/12 2004

Zhixin Yu: *Nanocatalysis. Mature Science Revisited or Something New*? 2005

Kjersti O. Christensen: *Synthesis gas from biomass*. 16/2 2005

Ingrid Aartun: *Non-conventional methods for producing olefins from ethane and propane*. 10/6 2005

Sølvi Storsæter: *Removal of NOx by catalytic processes*. 22/6 2005

Erlend Bjørgum: *Photocatalysis* 20/1 2006

Vidar Frøseth: *Catalytic upgrading of residues.* 16/6 2006

Florian Huber: *Catalysis in confined geometries – state of the art and relevance to industrial catalysis*. 2006

Øyvind Borg: *Challenges to catalysis in sustainable power generation from natural gas.* 27/4 2007.

Espen Standal Wangen: *Transportation fuels from biomass,* 25/5 2007

Hilde Dyrbeck: *Hydrogen storage in organic hydrides*. 2007

Svatopluk Chytil: *Synthesis and catalytic applications of mesoporous alumina*. 2007

Ingvar Kvande: *The role of catalysts in metal dusting*. 14/12 2007

Hilde Meland: *In situ/operando studies of working catalysts*. 23/5 2008.

Silje Fosse Håkonsen; *Catalysis in high temperature fuel cells*. 13/6 2008

Bjørn Christian Enger: *Synthesis and application of core-shell structured nanoparticles (CSNP) in catalysis.* 11/12 2008.

Nina Hammer: *Production of C_2 oxygenates from syngas*. 2008

Astrid Lervik Mejdell: *Recent advances in photocatalysis*. 8/5 2009.

Li He: *Conversion of algal-based biomass by thermochemical methods: opportunities and challenges*. 8/1 2010

Sara Boullosa Eiras: *Catalysts and materials development in solid oxide fuel cells*. 22/10 2010

Hamidreza Bakhtiary; *Production of C_2-C_4 alcohols from synthesis gas*. 3/11 2010.

Xuyen Kim Phan: *Direct catalytic conversion of carbohydrates to hydrocarbons*. 2011

Fatemeh Hayer: *Recent developments in the Fischer-Tropsch Synthesis over iron catalysts*. 15/3 2011

Shreyas Panduran Rane: *Catalytic Cleaning of Marine Fuel Exhaust Emissions*. 25/5 2001.

Fan Huang: *Catalysis in energy storage*. 17/9 2011

Oana Mihai: *Biomass conversion by pyrolysis and subsequent catalytic upgrading*. 7/9 2011

Jia Yang: *Carbide, Nitride and mixed oxide as replacements for noble metal catalysts*. 28/112011.

Nikolaosa E. Tsakoumis: *Recent progress in in situ vibrational spectroscopy for catalytic applications*. 18/11 2011.

Kazi Saima Sultana: *Catalytic conversion of CO_2.* 2011

Navaneethan Muthuswany: *Graphene, synthesis and energy related applications*. 9/12 2011.

Hassan Jamil Dar: *Compact steam reformers*. 2012.
Eleni Patanou*: Production of light olefins from syngas*. 2012

Paul Radstake: *Metal Nanoparticlers in Catalysis*. 14/12 2012

Ilya Gorelkin*: SCR-deNOx catalysis: Catalysis and processes for NOx removal from mobile sources.* 2013

Tayyaba Noor*: Catalytic combustions: catalysts and applications*. 2013

Ingvild Tronstad: *Thermal analysis: Principles, techniques and applications in catalyst characterization*. 2013

Fengliu Lou: *Challenges in large scale chemical and electrochemical energy storage.* 2013

Daham Sanjaya Gunawardana Panditha Vidana: *Mixed-metal oxide catalysts for ammonia oxidation.* 2014

Alexey Voronov: *Kinetic modeling of catalytic deNOx chemistry –state of art and recent progress in methodology and mechanistic insight.* 2014

Nicla Vicinanza: *Production of medium to high purity oxygen; an evaluation of alternative methods and applications*. 2014

Georg Voss: *Concepts and challenges in catalytic waste-water treatment.* 2014

Andreas Helland Lillebø: *Concepts for energy storage utilizing catalysis beyond Fischer-Tropsch synthesis.* 2014

Andrey Volynkin: *Catalytic oxidation of methane and other hydrocarbon in dilute mixtures*. 2015

Anh Hoang Dam: *The Principles of the Fluid Catalytic Cracking (FCC) Process – The Influence of Feedstock Quality, Reactor Technology and Operating Conditions.* 2015

Yanying Qi: *Catalysis for synthesis gas production and utilization, beyond FTS: state-of-the-art and reaction mechanisms. 2016*

Farbod Dadgar: *Electrocatalysis for electromobility - current status, challenges and future approaches to solve the catalytic limitations in batteries. 2016*

Xuehang Wang: *Recent progress in electrochemical production and conversion of hydrogen. 2016*

Alumni
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, Herøya

Sturla Vada
Isotopic transient kinetic investigations of catalytic reactions.
Defense of thesis: October 1994
Current position: Det norske, Trondheim

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, Trondheim

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, Trondheim

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, Stjørdal

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: Norsk Industri

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

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, Stavanger

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: Director, Downstream at Stratas Advisors, 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, Stavanger

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: Journalist, 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

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: Researcher, SINTEF

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: Post.doc. NTNU

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

Hamidreza Bakhtiary
Performance assessment of a packed bed microstructured reactor – heat exchanger for methanol synthesis from syngas.
Defense of thesis: November 2010
Current position: Xodus Group, Oslo

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

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

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: Assoc. Professor, NTNU

Nikolaos E. Tsakoumis
Deactivation of cobalt based Fischer-Tropsch synthesis catalysts
Defense of thesis: November 2011
Current position: Project coordinator. 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: Renjord AS. Trondheim

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:Project coordinator. NTNU

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

Ilya Viktorovich Gorelkin:
Concepts and models of the catalytic dehydrogenation of propane.
Defense of thesis: March 2013
Current position: Siemens, Trondheim

Tayyaba Noor
Sorption Enhanced Water Gas Shift Reaction: Materials and Catalysis.
Defense of thesis: June 2013
Current position: School of Chemical and Materials Engineering, SCME, NUST, Islamabad, Pakistan

Ingvild Tronstad
Corrosion of Copper and Oxidation of Dielectric Liquids in High Voltage Transformers.
Defense of thesis: June 2013
Current position: NAMMO Raufoss

Fengliu Lou
Aligned carbon nanotubes@manganese oxide coaxial arrays for lithium ion batteries.
Defense of thesis: September 2013

Current position: Post.doc. NTNU

Daham Sanjaya Gunawardana Panditha Vidana
Carbon formation phenomena and the initial stage of metal dusting corrosion - an experimental investigation
Defense of thesis: January 2014
Current position: Yara, Porsgrunn

Alexey Voronov
Sensitivity enhancement of X-ray absorption spechtroscopy applied to Co-based Fischer-Tropsch synthesis catalysts.
Defense of thesis: February 2014
Current position: Project Manager, Advanced Research Foundation, Division of Chemical, Biological and Medical investigations". Moscow, Russia

Nicla Vicinanza
An investigation of fundamental phenomena affecting the performance of sputtered Pd alloy thin film membranes for hydrogen separation
Defense of thesis: May 2014
Current position:

Georg Voss
Mesostructured alumina and the state of Ni as promotor for Co Fischer-Tropsch synthesis catalysts.
Defense of thesis: August 2014
Current position: Head of Laboratory, Department of Petroleum Engineering and Applied Geophysics, NTNU

Andreas Helland Lillebø
Conversion of biomass derived synthesis gas into liquid fuels via the Fischer-Tropsch synthesis process: Effect of alkali and alkaline earth metal impurities and CO conversional levels of cobal based catalysts.
Defense of thesis: September 2014
Current position: Cambi, Oslo

Andrey Volynkin
The role of carbon supports in platinum catalyzed hydrogenation/dehydrogenation model reaction.
Defend of thesis: September 1 2015
Current position: Institute of Marine Research, Bergen

Anh Hoang Dam
Bimetallic Catalyst System for Steam Reforming.
Defend of thesis: December 10 2015
Current position: Cealtech, Stavanger

Yanying Qi
Mechanistic Insights into Cobalt-based Fischer-Tropsch Synthesis.
Defend of thesis: April 25 2016
Current position: Post.doc. NTNU

Farbod Dadgar
Direct synthesis of dimethyl ether in microstructured reactors: The interactions between methanol synthesis and methanol dehydration
Defend of thesis: June 20 2016
Current position: Cambi, Oslo

Xuehang Wang
Porous carbon prepared by chemical activation for high-energy supercapacitors in ionic liquid electrolyte
Defend of thesis*:* September 30 2016
Current position: Post.doc.
Department of Materials Science and Engineering and A. J. Drexel Nanomaterials Institute, Drexel University, Philadelphia , PA 19104 USA