Annual Report

2017

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 Industry. As of January 2008 the centre has been established as a Gemini centre by NTNU and SINTEF.

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Annual Report 2017
KINCAT
Strong Point Centre Kinetics and Catalysis

Contents

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Academic staff:

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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 2017-31.12.17)

Laboratory personnel:

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Senior Engineer Estelle Vanhaecke

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Ole H. Bjørkedal
Endre Fenes
Ljubisa Gavrilovic
Xiaoyang Guo
Stine Lervold
Yahao Li
Shirley Elisabeth Liland
Juntian Niu
Eirik Østbye Pedersen
Joakim Tafjord
Martina Cazzolaro
Samuel Regli
Haakon Rui
Ata ul Rauf Salman
Marie Døvre Strømsheim
Yalan Wang
Cornelis Gerardus van der Wijst
Isaac Yeboah
Daniel Skodvin
Hongfei Ma
Jianyu Ma
Muhammad Zubair
Marthe Emelie Melandsø Buan

Postdoctoral fellows/Researchers 2017/2018

Qingjun Chen
Mari Helene Farstad
Li He
Jørgen Svendby
Yanying Qi
Marie Døvre Strømsheim
Xiang Feng
Diego Alexander Pena Zapata

Visitors 2017/2018

Wenyao Chen
Mehdi Mahmoodina
Katarzyna Swirk
Binga Mohan Larrasoana
Xiaoyang Guo

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

Harry T. Brun
Jan Morten Roel
Gunn Torill Wikdahl
Mikael Hammer
Erland Strendo

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

Research scientists:
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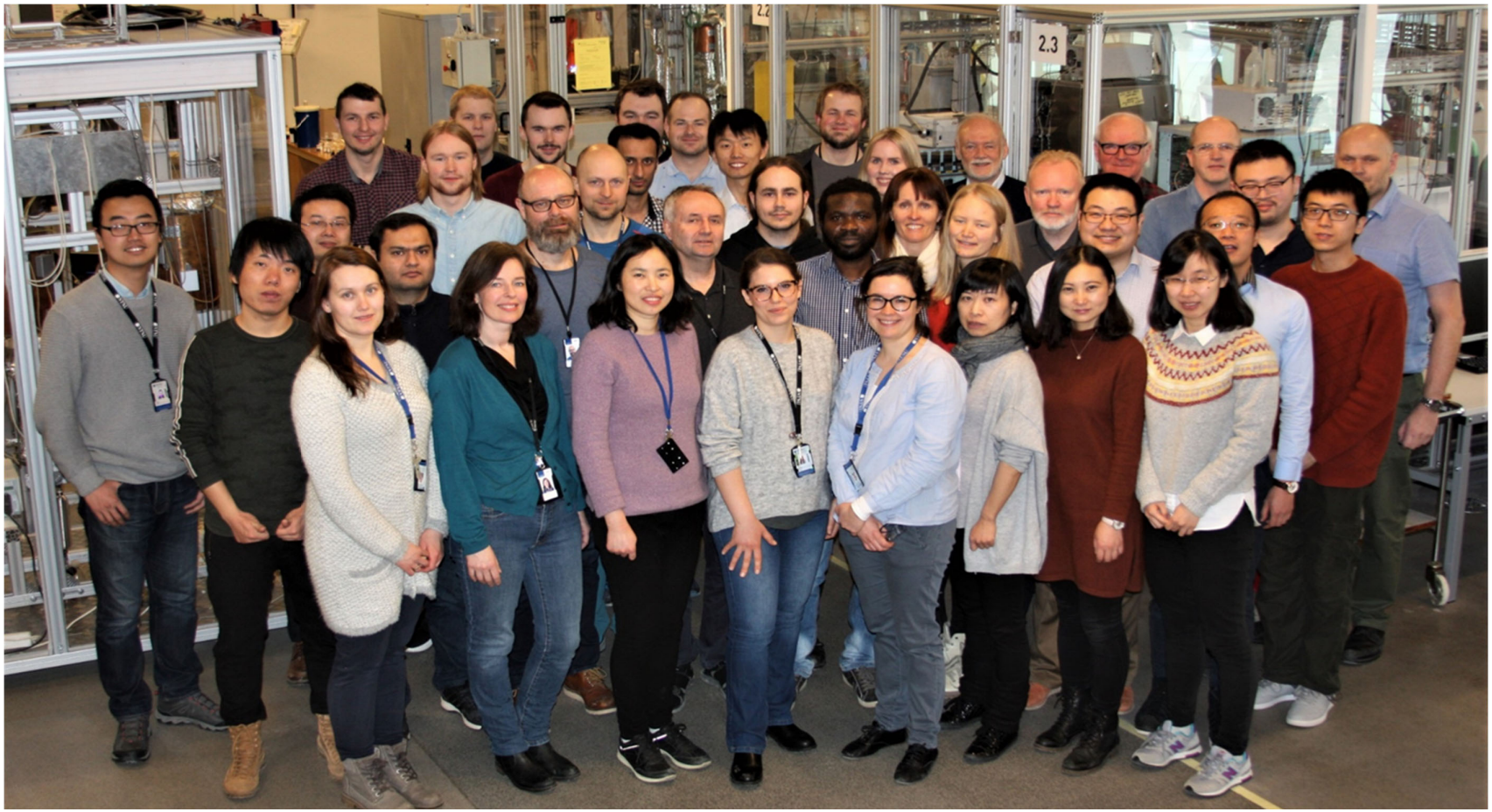
Research Scientist Hilde Bjørkan
Senior Scientist Bjørn Christian Enger
Senior Scientist Rune Lødeng
Research Scientist Rune Myrstad
Research Scientist Kumar R. Rout

Laboratory personnel
Senior Engineer Camilla Otterlei



4t[h] row: Ljubisa Gavrilovic, Jørgen Svendby, Joakim Tafjord, Ata ul Rauf Salman, Ole Bjørkedal, Samuel Regli, Endre Fenes, Erling Rytter, Anders Holmen, Rune Myrstad, Magnus Rønning
3[rd] row: Daniel Skodvin, Bjørn Christian Enger, Xiaoyang Guo, Stine Lervold, Edd Blekkan, Jianyu Ma
2[nd] row: Xiang Feng, Qingjun Chen, Muhammad Zubair, Håkon Bergem, Rune Lødeng, Eirik Pedersen, Isaac Yeboah, Hilde Venvik, Mari Helene Farstad, Yahao Li, Junitan Niu, Bingxu Chen
1[st] row: Hongfei Ma, Karin Dragsten, Camilla Otterlei, Jia Yang, Martina Cazzolaro, Estelle Vanhaecke, Li He, Yalan Wang, Yinyang Qi.
Not present: De Chen, Kjell Moljord, Shirley Liland, Haakon Rui, Marie Strømsheim, Cornelis van der Wijst, Torbjørn Gjervan, Hilde Bjørkan, Kumar Rout

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

❖ Industrial catalysis

- Oxychlorination
- Catalytic oxidation of NO to NO_2
- Catalytic oxidation of methanol to formaldehyde

❖ 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 liquefaction
- 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**

❖ **Gas cleaning**

- Sorbent and processes for H_2S removal.
- Sorbents and processes for CO_2 capture.

❖ **Photocatalysis**

- Water splitting
- Photoreforming

Main Laboratory Equipment

❖ Reaction Laboratories

- Small pilot plants for catalytic reforming/isomerization and hydrotreating/hydrocracking
- Small pilot plants for biomass conversion
- 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
- Granulation equipment

❖ 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 2017

- Three candidates completed their PhD degrees in 2017: Marthe Emelie Melandsø Buan, Ida Hjort and Marie Døvre Strømsheim. The titles of the dissertations and pictures of the candidates/committees/supervisors are enclosed.

- Eight M.Sc students completed their thesis in 2017. Their name and titles are enclosed.

- Professor Magnus Rønning was on a one year Sabbatical leave for 2016/ 2017 with Professor Jens Nørskov, Stanford University. USA. Professor De Chen is on a one year Sabbatical leave for 2017/2018 in China.

- iCSI – industrial Catalysis Science and Innovation – is a 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. A description of iCSI is enclosed.

- The Annual Meeting of ICSI was organized together with the Norwegian Catalysis Symposium on the 6th and 7th November 2017 at Hurdalsjøen Hotel. The program is enclosed.

- 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 Special Issue in Catalysis Today with selected papers from NGCS11 was finalized in 2017 with Hilde Venvik, Anders Holmen, De Chen, Erling Rytter and Duncan Akporiaye as Guest Editors.

- The group participates in several 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 scholarships 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.

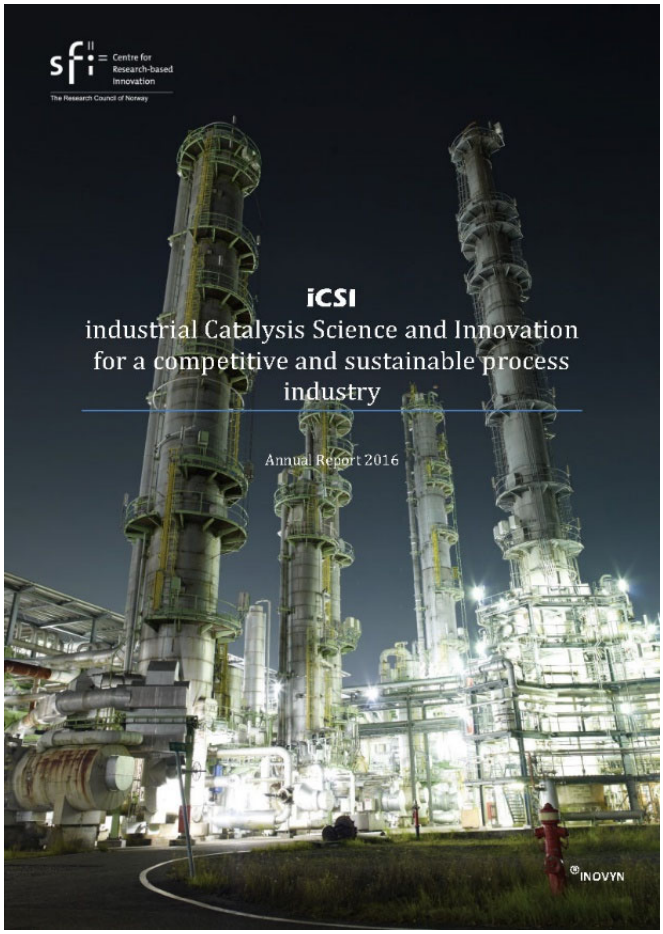
The iCSI Centre is pleased to announce the establishment of its ***Scientific Advisory Committee*** (SAC). Professor Alessandra Beretta (Politecnico di Milano), Professor Enrique Iglesia (UC Berkeley) and Professor Graham Hutchings (Cardiff University) are scientists from prominent institutions who have 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.
High surface area, surface acidity and thermal stability are regarded to be important properties for an SCR-catalyst. Ordered mesoporous alumina (OMA) prepared through a sol-gel synthesis may be a way to obtain these properties in a support material. Catalysts with Fe or Cu on an OMA-support have been synthesized and characterized. In-situ XAS/XRD experiments have been performed at the Swiss-Norwegian Beamline (SNBL) at ESRF in Grenoble to determine the state of the active metal during the SCR-reaction.
Furthermore, an SCR-testing unit have been designed and is currently under development with expected delivery in the spring of 2018. With this equipment in place, further kinetic studies may be performed.
The next step of the project will be to continue the screening of potential catalyst and enhance the synthesis procedure based on these results, as well as starting in depth-studies of kinetics and stability. A key parameter will be to achieve high activity in low temperature conditions.
Two students, Karoline Aasen Nilsen and Kin Hui, were included in the project for their specialization project the Autumn of 2018, and Kin Hui will continue with his master thesis as part of this project.

Presentations in 2017:

1. Bjørkedal, Ole Håvik; Rønning, Magnus; *Acid-modified mesoporous alumina as catalytic support for NH3-SCR*. Annual meeting for the Catalysis Division of the Norwegian Chemical Society; Hurdalssjøen; November 6^{th}-7^{th} 2017; Poster Presentation

Financial support:
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 2017:

1. N. Muthuswamy, M.E. Melandsø Buan, J.C. Walmsley, M. Rønning, Evaluation of ORR active sites in nitrogen-doped carbon nanofibers by KOH post treatment, *Catal. Today 321* (*2018) 11-16*
2. M.E. Melandsø Buan, N. Muthuswamy, J.C. Walmsley, D. Chen, M. Rønning, Nitrogen-doped Carbon Nanofibers for the Oxygen Reduction Reaction: Importance of Iron Growth Catalyst Phase, *ChemCatChem, 9, (2017) 1663 – 1674*
3. M.E. Melandsø Buan, A. Cognigni, J.C. Walmsley, N. Muthuswamy, M. Rønning, Active sites for the Oxygen Reduction Reaction in Nitrogen-doped Carbon Nanofibers, (2017) submitted
4. M.E Melandsø Buan, Nitrogen-doped Carbon Nanofibers for the Oxygen Reduction Reaction, PhD-thesis, defense 29.03.17

Presentions in 2017:

1. M.E.M. Buan, N. Muthuswamy, J.C. Walmsley, D. Chen, M. Rønning, Nitrogen-doped carbon nanofibers for oxygen reduction: The role of iron in forming active ORR sites, EUROPACAT 2107, August 27-31. 2017, Florence, Italy
2. M. Rønning, Nitrogen-doped carbon nanofibres: What are the requirements for application in PEM fuel cells?, Keynote lecture: CarboCat-VIII, June 26-29, 2018, Porto, Portugal

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

Development of stable Cu/C catalysts for selective hydrogenation of hydroxyacetone to 1,2-propanediol

Ph.D. Candidate: Martina Cazzolaro
Supervisor: Prof. De Chen
Co-supervisor: Assoc. Prof. Jia Yang

Pyrolysis is a thermochemical process assumed to become an avenue to petroleum-type products using renewable lignocellulosic biomass as feedstock. Catalytic hydrodeoxygenation (HDO) of bio-oil (the liquid product of pyrolysis) is one of the possible strategies to increase the hydrogen-carbon ratio, but the development of a highly active, selective and stable catalyst is still the main challenge. In this project, the selective hydrogenation of hydroxyacetone (HA), commonly present in bio-oil, to 1,2-propanediol (1,2-PDO), an added-value commodity chemical, will be used as simple model-reaction to study the HDO process.

Transition metal catalysts (mainly Ni- and/or Cu-based) showed good activity in bio-oil upgrading, but coke production resulted in shortened catalyst lifetime. Cu-based catalysts showed high activity also in the process of hydrogenolysis of glycerol to 1,2-PDO, that has HA as main intermediate: Cu particle size, dispersion and active area are the key parameters to control in order to achieve high activity and stability. Decrease of Cu active area, with particles agglomeration and formation of irregularly shaped clusters, is indeed reported as the main cause of deactivation.

This project aims to develop highly active and stable Cu-catalysts for 1,2-PDO production from HA. Since carbon supports have shown to be promising in terms of product selectivity, homemade carbon nanofibers, graphene and activated carbons will be used as catalyst supports. The interaction Cu-support will be tuned via chemical modification of the surface chemistry of the carbon supports. The properties of the prepared supports and catalysts will be carefully analyzed with various techniques: N_2 physisorption, N_2O chemisorption, H_2-TPR, TEM, XPS and XRD. The catalyst in powder form will be tested in a fixed-bed reactor in a lab-scale set-up; a GC-MS will be used to monitor activity, stability and selectivity of the catalysts towards the hydrogenation of HA to 1,2-PDO.

Financial support:
The project is funded by the Norwegian Research Council through the Bio4Fuels program.

Co-based Fischer−Tropsch Synthesis mechanism studied by density functional theory (DFT) using K adsorption as a probe

Post.doc: Dr. Qingjun Chen
Supervisor: Professor Edd A. Blekkan

In the Fischer–Tropsch synthesis (FTS) synthesis gas (CO + H_2) is converted into hydrocarbons, mainly n-alkanes and 1-alkenes. This is an attractive route for the production of chemicals and liquid fuels from natural gas, coal, and biomass. Cobalt-based FTS catalysts are preferred over their iron counterparts in gas-to-liquids processes due to their higher selectivity to paraffinic products, lower water gas shift activity, and longer lifetime. However, the activity of cobalt catalyst is very sensitive to inorganic pollutants, such as trace amounts of alkaline metals (such as K, Na), typical elements present in syngas from biomass gasification. Minor amounts of alkaline metals (100~1000 ppm) results in a significant decrease of the activity, without affecting the dispersion as measured by H_2 or CO chemisorption. This implies that the alkaline metals occupy sites on cobalt that are of particular importance for the catalytic activity. Therefore, K could also be used as the probe to study the active sites and CO activation mechanism of FTS on cobalt catalyst. In this work, the CO activation mechanism on Co surfaces was systematically studied by density functional theory (DFT) using K as a probe.

The equilibrium shape and exposed facets of hexagonal close-packed (hcp) Co were first calculated through a Wulff construction. 9 facets were exposed, and the energetics of K adsorption were calculated on every exposed facet. The results showed that K adsorption is favored on all facets, and that the B_5 site on a stepped facet (10-12) exhibits the highest adsorption energy (-2.41 eV), and thus is the most preferred site for K adsorption. K is very mobile on the surface, with low barriers against surface diffusion, except across steps.

Different CO activation routes were investigated. Activation energies and transition states were calculated on the stepped facet (10-12) and the typical flat facet (0001) with or without adsorbed K. On the flat facet (0001), the energy barrier of CO direct dissociation (CO→C+O) was found to be 2.41 eV, much higher than that of H-assisted CO dissociation. The H-assisted CO dissociation through the HCO route (2H+CO→HCO+H→HCOH→CH+OH) was found to have the lowest energy barrier of 1.41 eV. On the B_5 site of the stepped facet (10-12), the direct dissociation of CO was preferred, with an energy barrier of 1.14 eV, which was much lower than those on flat the facet (0001). This indicates that the B_5 site on the stepped facet (10-12) might play a crucial role in CO activation and FTS on hcp Co. Furthermore, pre-adsorbed K caused a slight increase in the CO dissociation barrier on the (0001) facet, but had almost no effect on the CO dissociation barriers on the stepped facet (10-12). We propose that blocking the active B_5 site on the stepped facet (10-12) by K is the main cause of the activity loss of the cobalt catalyst following K adsorption. It is also noted that pre-adsorbed K improves CO adsorption and slightly inhibits H adsorption on hcp Co. This could explain observed selectivity changes (reduced CH_4 selectivity) following K poisoning of cobalt catalysts.

Publications and Presentations in 2017:

1. 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*, *Phys. Chem. Chem. Phys.* 2017, 19, 12246.
2. Qingjun Chen, Ingeborg-Helene Svenum, Yanying Qi, Ljubisa Gavrilovic, De Chen, Anders Holmen, Edd A. Blekkan, *CO activation mechanism of Fischer−Tropsch*

Synthesis on hcp Co studied by density functional theory (DFT) using K adsorption as a probe, the 13th European Congress on Catalysis (EUROPACAT 2017), *Oral Presentation*, Florence, Italy, August 28-31, 2017.

Financial Support:
This project is financed by the ENERGIX programme contract no: 10417501.

Co(11-20) and Pd3Au(100) single crystals as catalyst model systems

Ph.D. Candidate: Marie D. Strømsheim

Supervisor: Professor Hilde Johnsen Venvik

Co-supervisors: Professor Anne Borg, Department of Physics, NTNU, and Research Scientist Dr. Ingeborg-Helene Svenum, SINTEF Industry

Single crystals provide model systems that can further the understanding of phenomena occuring at the surface of a catalyst e.g adsorption/desorption, reaction, surface segregation, promotion and poisoning. Understanding the dynamic surface of a cobalt (Co)-based Fischer Tropsch catalyst motivated the work with a Co single crystal, and the work with a Pd-alloy single crystal was motivated by understanding the segregation behavior of the alloying element in Pd-based catalysts and membranes under relevant conditions.

The surface of Co(11-20) is known from previous work in the group to reconstruct upon exposure to CO at room temperature. Therefore the Co(11-20) surface was chosen as the model system for Co-based Fischer – Tropsch catalysts for conversion of natural gas or biomass into liqiuid fuels. Previous experiments at KinCat also reported a significant decrease in the catalytic activity for Co-based catalysts with 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 such as CO adsorption and hydrocarbon adsorption and decomposition, were studied using Low Energy Electron Diffraction (LEED), Scanning Tunneling Microscopy (STM), and High resolution x-ray photoelectron spectroscopy (HRXPS). Density functional theory (DFT) calculations were also performed to complement the experimental findings.

The previous STM results showed that adsorption of CO ($\sim 1 \cdot 10^{-9}$ 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. A similar experiment with pre-deposited submonolayer amounts of potassium (K), 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.

The formation of a (2x5) carbon overlayer on Co(11-20) occurs upon exposure to C_2H_4 at 470-520 K. The accumulation of detrimental carbon has been identified as possible deactivation mechanism by Moodley et al. Therefore the adsorption and decomposition of C_2H_4 on the Co(11-20) surface without and with submonolayer amounts of K was investigated. While the overlayer formed on both the clean and the K-covered surface, significant differences were

found for the C_2H_4 adsorption and decomposition. Heating the carbon overlayer on the clean cobalt surface to 370°C resulted in the formation of graphitic carbon, and a loss of the (2x5) structure. This did not occur for the K-covered surface, although a possible transition from carbidic to graphitic carbon at a temperature higher than 380°C can not be excluded.

Palladium (Pd) based catalysts are often applied in oxidation and hydrogenation reactions, and Ag, Cu and Au as alloying elements 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 was found to form on $Pd_3Au(100)$, similar to Pd(100) and $Pd_{75}Ag_{25}(100)$, upon oxygen exposure of 10^{-3} mbar, and ~310° C under UHV conditions. To further elucidate the effect of Au as an alloying element, CO oxidation over $Pd_3Au(100)$ was studied with a combination of 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 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 $Pd_{75}Ag_{25}(100)$. Furthermore, $Pd_3Au(100)$ does not display reversed hysteresis, as was the case for $Pd_{75}Ag_{25}(100)$. However, similarly to $Pd_{75}Ag_{25}(100)$, the results indicate less long range order of the surface oxide in comparison to pure Pd, and the concurrent presence of chemisorbed oxygen with the surface oxide. Thus, Au as an alloying element results in different behavior in comparison to Ag, and only minor changes to the pure Pd surface in terms of active phase and hysteresis behavior.

Financial support:
The research has been performed with financial support from NTNU and the Centre for research-based innovation (SFI) inGAP (Innovative Natural Gas Processes and Products) appointed by the Research Council of Norway (Project no. 174893/O30) for the period 2007-2015, and Statoil ASA through the Gas Technology Centre (NTNU-SINTEF). Partners in inGAP include the University of Oslo (UiO), the Norwegian University of Science and Technology (NTNU), SINTEF, Statoil, Haldor Topsøe AS and INEOS.

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 NN9355k, and local resources on Vilje, account no. ntnu946.

Publications and presentations**:**

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)"* Topics in Catalysis, 2017, Volume 60, Issue 17–18, pp 1439–1448

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)"*
Catalysis Today, Volume 299, 2018, Pages 37-46

Marie D. Strømsheim, *Co(11-20) and Pd3Au(100) single crystals as catalyst model systems*, PhD-thesis, defence 13.12.2017

Material degradation by metal dusting corrosion in compact reformer concepts

Ph.D. Candidate: Xiaoyang Guo
Supervisor: Prof. Hilde Johnsen Venvik
Co-supervisors: Prof. De Chen, Senior Scientist John Walmsley, Senior Scientist Per Erik Vullum and Dr. Estelle Vanhaecke

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 are needed to avoid catastrophic events. Micro-structured 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 a more severe issue than in conventional reactor vessels.

Ni-based Inconel 601 alloy samples were pre-oxidized in 10% steam in Ar at 540˚C before exposure to different carburizing atmospheres. Auger depth profile indicate the thickness of the oxide layer formed by pre-oxidization is around 45 nm and rich in Cr, O and Fe, which is in accordance with Raman scattering spectra. The metal dusting conditions after oxidization for exposure times from 1h to 20h are either 1 bar and 10% CO in Ar at 750 ˚C (infinite a_c), or a 20% CO syngas mixture (finite a_c). SEM images of alloy sample exposed to infinite carbon activity show fewer and shorter carbon filaments compared to the samples exposed to the more industrially relevant finite low carbon activity. X-ray diffraction results from these two series samples indicate that Inconel 601 exposed to 10% CO in Ar develops more surface Cr_2O_3, while when exposed to 20% CO more $(Ni, Fe, Cr)_3O_4$ spinel phase is formed. The spinel is not stable under syngas and can be reduced to metal particles acting as catalyst for carbon deposition. Raman scattering spectra confirms that for increasing 10% CO exposure time, the intensity ratio of Cr_2O_3 to spinel increases. This indicates that Cr atoms were able to diffuse towards the surface to form protective Cr_2O_3. For the sample exposed to 20% CO syngas the spinel phase is always dominant in the Raman spectra. The intensity ratio of D-band to G-band (I_D/I_G) grows from 1.01 for 1h to 1.64 over 20h, which indicates that disordered carbon grows faster than ordered carbon. A shoulder peak next to the G band (D' band) is another sign of highly disordered carbon.

Publications and presentations in 2017:

1. Xiaoyang Guo; P.V.D.S. Gunawardana; De Chen; Estelle Vanhaecke; Hilde J. Venvik; John C. Walmsley. *Investigation of Metal Dusting Corrosion Process over UNS N08800 Alloy* CORROSION 2017 (NACE international) ISBN: 9781510840348
2. Xiaoyang Guo; P.V.D.S. Gunawardana; De Chen; Estelle Vanhaecke; Hilde J. Venvik; John C. Walmsley. *Investigation of Metal Dusting Corrosion Process over UNS N08800 Alloy* CORROSION 2017 (NACE international) 26-30 March, New Orleans, Louisiana, USA. Oral presentation.
3. Xiaoyang Guo; Estelle Vanhaecke; Jianyu Ma; P.V.D.S. Gunawardana; John C. Walmsley; De Chen and Hilde J. Venvik. *Investigation of initial stage of Metal Dusting Corrosion Process over Inconel 601* EUROCORR2017 20th International Corrosion Congress & Process Safety Congress 2017 Prague Czech Republic 3-7 September 2017. Oral presentation.

4. Xiaoyang Guo; P.V.D.S. Gunawardana; De Chen; Estelle Vanhaecke; Hilde J. Venvik; John C. Walmsley. *Characterization of metal dusting corrosion on instrumentation used in natural gas conversion technologies* NNUM 2017 Nordic Nanolab User Meeting 2017 9-10 May Trondheim Norway. Poster.
5. Medvedovski, Eugene; Ma, Jianyu; Guo, Xiaoyang; Vanhaecke, Estelle; Venvik, Hilde Johnsen. *Studies of Corrosion Resistance of Aluminized Coatings in Metal Dusting Environments* Materials Science & Technology 2017 08-12 October Pittsburgh, PA, USA Oral presentation.
6. Xiaoyang Guo, Estelle Vanhaecke, Per Erik Vullum, John C. Walmsley, De. Chen, Hilde J. Venvik *Suppressed carbon formation on Fe-Ni based high temperature alloys.* Norwegian Catalysis Symposium 2017 6-7 November Oslo Norway. Poster.

Financial support:
The project is funded by the Research Council of Norway under the GASSMAKS research program (Contract No.233869/E30)

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, selectivity and stability is investigated with an operando study, combining mass- and UV-Vis-NIR spectrometry during both transient and steady state experiments. This approach have increased our understanding of the catalytic system and the underlying principles that guide catalyst properties. Additional characterization techniques as infrared-, Raman- and x-ray photoelectron spectroscopy was attempted. The work was presented at two international conferences: NAM 25 and Europacat 2017.

During the year, three months was dedicated to a literature study on kinetic models for partial oxidation reactions, funded by a grant from the EUROKIN consortium. The project resulted in two internal presentations and a written report and the experience gained new ideas to attempt in ethylene oxychlorination.

Presentations/publications in 2017:

1. E. Fenes, M. F. Baidoo, K. R. Rout, T. Fuglerud, D. Chen: Rational Design of $CuCl_2/Al_2O_3$ based Oxychlorination Catalysts. NAM25: North American Catalysis Society Meeting 2017

2. M. F. Baidoo, E. Fenes, K. R. Rout, T. Fuglerud, D. Chen: On the effects of K and La co-promotion on $CuCl_2/\gamma$-Al_2O_3 catalysts for the oxychlorination of ethylene. *Catalysis Today, 2017, 299. 164-171*
3. 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, 2017, 352, 218-228*
4. E. Fenes, K. R. Rout, M.F. Baidoo, T. Fuglerud, D. Chen: First Ionization energy as Descriptor of Alkali Metal Promoted Cu-based Oxychlorination Catalysts, Europacat 2017, Florence
5. E. Fenes, M. F. Baidoo, K. R. Rout, T. Fuglerud, D. Chen: Rational catalyst design in ethylene oxychlorination: alkali promotion, activity descriptors and rate diagrams, iCSI annual meeting 2017, Hurdalsjøen

Financial support:
iCSI - Industrial Catalysis Science and Innovation

Investigations of the methanol to formaldehyde (MTF) reaction over silver

Ph.D. Candidate: Stine Lervold
Supervisor: Prof. Hilde J. Venvik
Co-supervisors: Associate Professor Jia Yang and Senior Researcher Dr.ing Rune Lødeng (SINTEF).

Formaldehyde is the essential component of wood adhesives for a wide range of applications and an important intermediate 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, isothermal conditions and potentially negligible mass transport limitations and gas phase reactions.

Presentations in 2017:

1. Stine Lervold, Nikolas Beck, Rune Lødeng, Jia Yang, Kristin Bingen, Terje Pedersen, Hilde J. Venvik. *IIA3-WP3.1: Annular reactor for investigation of the Methanol to*

Formaldehyde (MTF) reaction. iCSI Annual Meeting, Hurdalsjøen, Norway, 2017. Oral presentation.

Financial support:
The project is a research activity (IIA3, WP3.1) 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.

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 (SINTEF)

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).

For both reactions several Ni-Co based catalysts supported on a hydrotalcite-structure has been studied. For the SR reaction it has been found that the bimetallic Ni-Co catalyst severely enhances the activity compared to pure Ni and pure Co. The same catalysts have also been investigated for the total combustion reaction, as this reaction is also relevant for methane decomposition. Here it was found that pure Co is the most active. Including in the total combustion reaction experiment a UV-vis-NIR spectroscopy was used to collect in-situ information on the oxidation state of the active metals, the idea is to use this oxidation state knowledge to improve the catalysts even further using promoters. 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.

Publications and presentations in 2017

1. Liland, Shirley Elisabeth; Rout, Kumar Ranjan; Fenes, Endre; Yang, Jia; Chen, De. Rational Design of Ni-Co/Hydrotalcite Catalyst for Methane Total Combustion using operando UV-Vis spectroscopy. Norwegian Catalysis Symposium 2017. November 6-7th 2017, Hurdal, Norway
2. Liland, Shirley Elisabeth; Wang, Yalan; Qi, Yanying; Rout, Kumar Ranjan; Chen, De. Unprecedented Active and Stable Ni-Co Bimetallic Catalyst for Steam Methane

Reforming: Combined DFT, Microkinetic Analysis and Kinetic Study. North American Catalysis Society Meeting. June 4-9th, 2017, Denver, USA
3. Wang, Hongmin; Blaylock, D. Wayne; Dam, Anh Hoang; Liland, Shirley Elisabeth; Rout, Kumar Ranjan; Zhu, Yi-An; Green, William H.; Holmen, Anders; Chen, De. Steam methane reforming on a Ni-based bimetallic catalyst: Density functional theory and experimental studies of the catalytic consequence of surface alloying of Ni with Ag. *Catalysis science & technology* 2017 ;Volume 7.(8) s. 1713-1725

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

Impact of promoters and support on Cu mobility in $CuCl_2$ based oxychlorination catalysts

Ph.D. Candidate: Hongfei Ma
Supervisor: Prof. De Chen
Co-supervisor: Dr Kumar Ranjan Rout & Terje Fuglerud

Vinyl chloride monomer (VCM) is the monomer in poly vinyl chloride (PVC) which is one of the most commonly used plastics and has a wide range of applications in our daily life, for example in construction materials, clothes and electronics. As a result, there is a high demand and over 40 million tons of PVC are produced every year, leading to VCM being a very valuable chemical. VCM is produced from ethylene and chlorine in a process involving several conversion steps. Oxychlorination of ethylene, producing ethylene dichloride (EDC) from ethylene, HCl and oxygen in a catalytic gas phase reactor, is used to recycle the HCl formed during EDC cracking. In addition, selective chlorination and hydrogenation are used actively to control the composition of process streams with the aim of improving process efficiency and reduce process equipment fouling.

In this project, promoters such as K and Mg, are employed to modify the performance of the copper-alumina catalyst and investigated by combining mass spectrometry and operando or in situ techniques such as UV-Vis spectroscopy. By using those techniques, we try to establish methods for *in situ* studies of Cu migration, byproduct- and carbon formation in order to understand the deactivation mechanisms of $CuCl_2$ based catalysts through kinetic studies.

Since starting my PhD in middle of November, I have already familiarized myself with the existing equipment and literature in addition to produce catalysts and performing step transient, steady-state and temperature programmed experiments. Based on these experiments, an abstract to the 18th Nordic Symposium on Catalysis is in preparation. We are currently designing and building a new setup in order to further this work in 2018.

Financial support:
The project is a research activity under iCSI-industrial Catalysis Science and Innovation.

Chemical Looping Desulfurization

Ph.D. Candidate: Jianyu Ma
Supervisor: Professor Edd A. Blekkan
Co-supervisor: Dr. Kumar R. Rout, SINTEF.

Bioenergy is a significant contributor to the renewable energy supply in Norway. Syngas from biomass gasification can be used for electricity production or as a feedstock in chemical synthesis to produce synthetic fuels. The gas is a complex mixture including H_2, CO, H_2O, as well as S containing species, which may lead to H_2S formation and lead to corrosion or poisoning catalysts in downstream process steps. Hence, removal of sulphur from the syngas is important for all applications of the syngas.

The Chemical Looping Desulphurization project (CLD), focuses on using Mn-based high temperature solid sorbent (HTSS) for desulphurization in a novel reactor system. Sulfur removal from the syngas from biomass gasification by HTSS represents a promising and energy efficient method. Mn-based solid sorbents are promising HTSS for sulfur removal due to several beneficial including low cost. The aim of the project is to solve key technological issues and placing this technology within the portfolio of cost-effective S capture technologies.

The research topic includes development of chemically- and mechanically stable Mn-based HTSS spherical pellets, and developing a kinetic model for sulfurization/de-sulfurization based on a non-catalytic gas-solid reaction mechanism. The work is part of a larger project (collaboration with SINTEF), where the results will be used in developing a new reactor and process for gas cleaning.

Publications in 2017:

S.Chytil, M. Kure, R.Lødeng, E.A Blekkan, Performance of Mn-based H2S sorbents in dry, reducing atmosphere – Manganese oxide support effects, Fuel, 196 (2017), 124-133.

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
Co-supervisors: Prof. De Chen, Dr. Ingeborg Helene Svenum (SINTEF)

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, 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 is studied, particularly the role of the Co-MnO interface.

Presentations in 2017:

1. Østbye Pedersen, Eirik; Svenum, Ingeborg-Helene; Blekkan, Edd. A. Mn promotion effects in Co-based Fischer-Tropsch production of light olefins. Poster presentation, 16th Norwegian catalysis symposium, 6.11.2017-7.11.2011, Hurdalssjøen, Norway.
2. Østbye Pedersen, Eirik; Svenum, Ingeborg-Helene; Blekkan, Edd. A. Mn promotion effects in Co-based Fischer-Tropsch production of light olefins. Poster presentation, 13th European Congress on Catalysis, 27.8.2017-31.08.2011, Florence, Italy.

Financial support:
The Norwegian Research Council, contract no. 224968/E30 under the Gassmaks programme. Computational resources provided by UNINETT Sigma2 under project no. NN9336K.

Reaction mechanism investigation by combined DFT calculations and microkinetic modelling

Post.doc: Yanying Qi
Supervisors: Prof. De Chen

The partial oxidation of methanol to formaldehyde is an important industrial process due to the versatility of formaldehyde as an intermediate in chemical synthesis. The adsorption energies of main species in catalytic reaction of partial oxidation of methanol on Ag (211) and Ag (111) are calculated and it is found that the adsorption on Ag (211) are stronger. Moreover, microkinetic modelling was performed to investigate the reaction mechanism of formaldehyde formation and predict information about surface coverages under reaction conditions and relative rates of various elementary steps. It is proved that oxygen could facility the reaction activity and selectivity simultaneously compared to direct dissociation of methanol.

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. It is found that alkali metals, such as K, Na, and/or rare earth metals like La as promoters increase the activity-, selectivity- and stability of CuCl2 based catalysts by kinetic studies. In this year, the promoter (i.e. K and Na) effect on ethylene adsorption in catalytic

oxychlorination of ethylene were investigated and Bader charge analysis and analysis of charge density difference during K/Na absorbs on the surface were performed. It is found that co-adsorbed K/Na change the electronic distribution of $CuCl_2$ surface and enhance ethylene adsorption slightly. The adsorption energy of ethylene on surface with co-adsorbed K/KCl can correlate to the charge change of surface Cu rather than Cl.

The effect of water on selectivity in formaldehyde formation will be studied by combined DFT calculation and microkinetic modelling. The promoter (i.e. K and Na) effect on oxychlorination of ethylene will be investigated further.

Publications in 2017:

1. Y. Qi, C. Ledesma, J. Yang, X. Duan, Y. Zhu, D. Chen, A. Holmen. J. Catal. 2017, 349,110-117
2. Q. Chen, I. Svenum; Y. Qi, L. Gavrilovic, D. Chen, A. Holmen, E. Blekkan. Phys. Chem. Chem. Phys., 2017, 19, 12246-12254

Financial support:
The project is funded by center for industrial Catalysis Science and Innovation (iCSI).

Advanced *operando* characterisation of catalysts for sustainable process industries

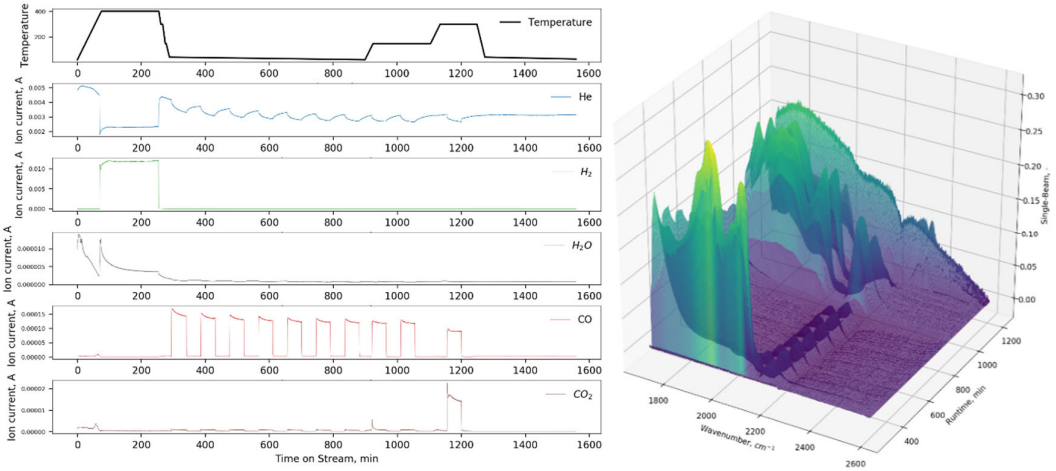
Ph.D. Candidate: Samuel K. Regli
Supervisor: Prof. Magnus Rønning
Co-Supervisor: Prof. Hilde J. Venvik

This PhD project is part of the industrial Catalysis Science and Innovation (iCSI) centre. 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 involved industrial partners supply key sectors of the global market (catalysts, chemicals, fertilizers, 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 prediction of the kinetically relevant steps. Moreover, the combined approach could significantly improve the parameter reliability by direct measurement of adsorption parameters in kinetic models.

Key characterisation techniques in this project are X-ray absorption spectroscopy with synchrotron radiation, X-ray diffraction, Fourier-transform infrared spectroscopy and Raman spectroscopy. The combination thereof allows for simultaneous *in situ* measurements of both bulk and surface of the catalyst as well as the product stream during operation at industrially relevant conditions, with temperatures of 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 favourable compositions and conditions enabling processes with higher efficiency, lower energy consumption and improved lifetime.



Example of DRIFTS study of time resolved in situ adsorption and desorption of carbon monoxide in helium on Ni on Hydrotalcite at different temperatures over time with monitoring of downstream composition with mass spectrometry.

Presentations 2017

1. M. Rønning, *In situ characterisation of catalysts without compromising process conditions,* Keynote lecture, ESRF User Meeting 2017, February 6-8 2017, Grenoble, France
2. M. Rønning, *Combining in situ characterization techniques to reveal real-time deactivation mechanisms in Fischer-Tropsch synthesis catalysts,* 253rd ACS National Meeting, April 2-6, 2017, San Francisco, USA

Financial Support:
This project is funded through the Research Council of Norway (NFR) through the industrial Catalysis Science and Innovation centre.

Catalysts for attaining NO/NO_2 equilibrium

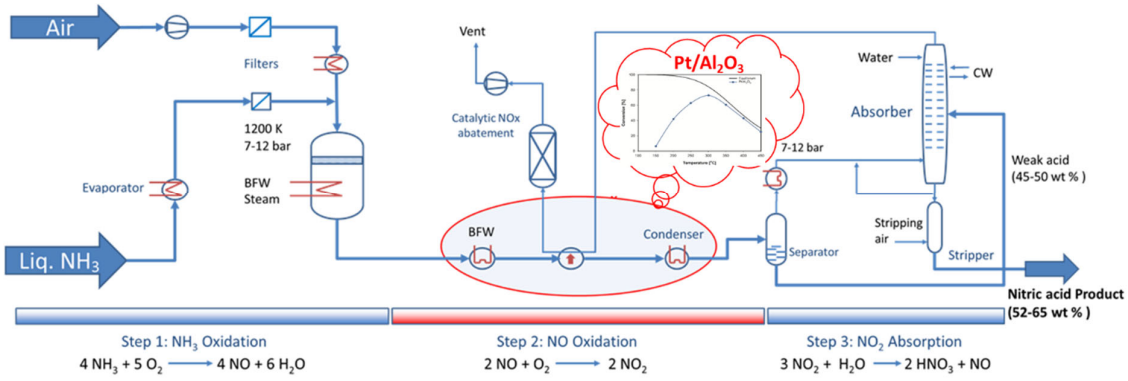
Ph.D. Candidate: Ata ul Rauf Salman
Supervisor: Professor Magnus Rønning,
Co-supervisors: Dr. Rune Lødeng, Dr. Bjørn Christian Enger

Nitric acid is an important industrial chemical. Commercial production of nitric acid takes place via the Ostwald process. The objective of the project is to develop an active catalyst to fully oxidize NO to NO_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°C has the potential of 15 % additional heat recovery from the NO oxidation process. The project is carried out in collaboration with the Yara Technology Centre.

An experimental setup capable of testing catalyst for NO oxidation under industrial conditions was designed and built. 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.
Catalytic oxidation of nitric oxide, over supported platinum catalyzing, using a dry feed (10% NO, 6% O_2) was studied. A kinetic model was established, an apparent activation energy and reaction orders were calculated. A reaction mechanism was proposed based on observed experimental results and rate equation.

Several other catalytic materials (mixed metal oxides) are currently under investigation for NO oxidation. Promising catalysts will be tested in wet feed (15% H_2O).



Process flow diagram of a single pressure nitric acid plant indicating substitution of gas phase NO oxidation with a compact Pt/Al_2O_3 catalytic converter.

Publications in 2017:

1. A.u.R. Salman, X. Auvray, B.C. Enger, R. Lødeng, M. Menon, D. Waller, M. Rønning, Catalytic oxidation of NO to NO_2 for nitric acid production over a Pt/Al_2O_3 catalyst, *(2017) submitted*

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.

Carbon Nanomaterial-Ionic Liquid Hybrid for Ultrahigh Energy Supercapacitor

Ph.D. Candidate: Daniel Skodvin
Supervisor: Prof. De Chen
Co-Supervisor: Dr. Qingjun Chen

The desire to use more renewable energy has made energy storage and conversion one of the greatest challenges in today's society. Energy needs to be stored more efficiently, thus improvements in the energy density of supercapacitors (SCs) should be achieved in order to

meet today's requirements. In this research, mesoporous carbon nanospheres are synthesized and used as electrode material in SCs using ionic liquids. The main objective is to develop SCs with high energy density (> 80 Wh/kg) and specific power (> 10 kW/kg). In addition, a high specific capacitance of 600 F/g should be realized using an operating voltage window of 4 V. This could be achieved by maximizing the ion packing density in the nanopores. In addition, the amount of mesopores in the carbon materials should be maximized, since mesopores provide low resistance during ion transport. Mesoporous carbon materials should have high specific surface areas (> 3000 m^2/g) and pore volumes (> 2 cm^3/g), which will provide a high ion packing ability. This could be realized by a careful study of the activation procedure, where several activating agents, including CO_2, ammonia and steam, will be used in order to optimize the pore size distribution of the carbon material.

Another objective of this work is to prepare cheaper and more environmentally friendly carbon materials to be applied in SCs. Lignin, which is an inexpensive, nontoxic and abundant renewable aromatic biopolymer, could be a promising precursor in the synthesis of mesoporous carbon nanospheres. To date, a maximum specific capacitance of 444 F/g using an operating voltage window of 4 V has been achieved in this work. Achieving these goals would enable a wide application range in the energy sector and improve renewable energy storage and conversion. This project could promote the use of renewable energy in the public transportation sector.

Financial Support:
The project is funded by the Research Council of Norway.

Biopolymer-mediated synthesis of Fe catalysts for the Fischer Tropsch synthesis based on renewable feedstocks

Ph.D. Candidate: Joakim Tafjord
Supervisor: Ass. Prof. Jia Yang
Co-supervisors: Prof. Anders Holmen and Research Scientist Rune Myrstad

The depletion of oil reserves has increased the interest in developing and improving processes that can replace the use of crude oil. An alternative is the Fischer Tropsch synthesis (FTS), a catalytic process where syngas ($CO+H_2$) reacts to form a range of hydrocarbons, such as light olefins, gasoline, diesel and waxes. The lower olefins (C_2-C_4) and their derivatives are important building blocks in the chemical industry, where they are used to produce many high performance materials and chemical products, i.e. plastic and engineering resins, lubricants, coatings and paints. To increase the renewability of the process, the syngas feedstock should derive from biomass. However, syngas from biomass is lean in hydrogen, and can be rich in CO_2 if extensive removal is not performed. In this case, iron is an attractive catalyst, as it can manage a relatively wide range of syngas feed ratios (H_2/CO = 0.5-2.5), due to the water-gas-shift reaction, where CO_2 also plays a role. In addition can also work at higher temperatures with low methane production. However, iron catalyst are prone to deactivation by sintering, catalyst attrition, phase-transformations and carbon deposition.

This project aims at synthesizing novel iron-based catalysts that is less susceptible to deactivation. The method involves the use of biopolymers, followed by pyrolysis, to form a carbon support for iron nanoparticles. Synthesis conditions will be varied to produce a catalyst with monodisperse iron nanoparticles, while maintaining a support with satisfying porosity. Powder XRD, S(T)EM and TEM will be used to determine iron particle size,

distribution and morphology, and BET to measure the porosity of the catalyst. The catalyst performance, stability and selectivity towards lower olefins will be investigated in the high-pressure FT rig, whereas mechanistic insights will be obtained by SSTIKA.

Financial support:
Faculty of Natural Sciences, Norwegian University of Science and Technology (NTNU)

Descriptor-based microkinetic analysis of Fischer-Tropsch synthesis towards light olefins production

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

Fischer-Tropsch synthesis (FTS) is a process for producing hydrocarbons and oxygenates by converting synthesis gas generated from coal, natural gas and biomass. Light olefins (C2 - C4 olefins) production directly from FTS has drawing increasing attention, because of extensively used of light olefins in the chemical industry as key building blocks. Although the F-T synthesis has been applied in industry for decades since discovered in the 1920s, the exact reaction mechanism is still under debate. In this work, a descriptor-based microkinetic analysis was preformed to investigate the mechanisms of FTS towards light olefins production. The strategy that using a hybrid semiempirical approach to fast predict surface reaction energetics was proposed herein, with C-, H- and O-metal binding energy as three sole descriptors. Adsorption energies were estimated by an improved UBI-QEP (unity bond index-quadratic exponential potential) method, which could satisfactorily fit the DFT calculated values. Brønsted-Evans-Polanyi (BEP) relationships were applied to obtain activation energies. The hybrid semiempirical approach (modified UBI-QEP + BEP) reduces radically the computational expenses, but keeps accuracy compared to DFT computations. The quickly generated energetics was then utilized in microkinetic modeling for FTS, with which we gained better understanding of reaction mechanisms and screened high activity catalysts. The predicted relatively high activity catalysts for light olefins production In FTS are Co, Ru and Iron carbide, among 8 transition metals (Co, Ru, Fe, Ni, Rh, Pt, Pd and Cu), under conditions: T = 483 K, P = 1.85 bar, $H_2/CO = 2$, consistent with experiments. Microkinetic modeling results also indicate that Mn has very little influence on Co activity for C_2H_4 and C_3H_6 formation, while K suppresses Co activity for C_2H_4 and C_3H_6 production apparently. CO activation mainly occurs via hydrogen-assisted CO dissociation. The major chain growth takes place through the coupling of CH+CO and CH3+CO pathways.

Publications and presentations in 2017:

1. Y. Wang, L. Xiao, Y. Qi, Y. Zhu and D. Chen, Strategy to Rapidly Screen Heterogeneous Transition Metal Catalysts: Microkinetic Analysis of Steam Methane Reforming from Combined DFT Calculations and UBI-QEP Method. Oral presentation. North American Catalysis Society Meeting 2017, Denver, USA. June 4-9, 2017.
2. Y. Wang, L. Xiao, Y. Qi, S. E. Liland, K. R. Rout, Y. Zhu, J. Yang, D. Chen, and A. Holmen, Microkinetic analysis of steam methane reforming over transition metal surfaces: Combined DFT calculations and UBI-QEP method. Oral presentation. Europacat 2017, Florence, Italy. August 27-31, 2017.

3. Y. Wang, L. Xiao, Y. Qi, Y. Zhu, J. Yang, D. Chen, A. Holmen, Microkinetic analysis of light olefins production from synthesis gas: Combined UBI-QEP method and BEP relationship. Poster presentation. Norwegian Catalysis Symposium 2017, Oslo, Norway. November 6-7, 2017.

Integrated H_2BioOil process for efficient biofuel production

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

Interest in renewable energy and fuel sources has spiked over the decades due to the over dependence on fossil fuel for transport fuel. Although, there are several paths to convert solid biomass to fuel to date no sustainable route has matured. Bio-oil produced from pyrolysis or liquefaction of woody biomass seem promising route towards sustainable Biorefinery concept. 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 and hydrodeoxygenation (HDO) reactions will be optimized on cheaply and rationally designed Cu and Ni based catalyst supported on TiO_2 as upstream bed, in tandem with $MoXP/Al_2O_3$ where X (Ni, Fe, Co, Mn, Ru etc.) as downstream bed. Therefore, a rationally catalyst design based on oxophilicity trend of transitional metals will be applied. 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.

Presentation in 2017:

1. I. Yeboah, K. R. Rout, X. Duan [c] and D. Chen, *A tandem aldol and hydrodeoxygenation (HDO) reactions of Bio-Oil oxygenates fraction to hydrocarbon*, NAM2017, Denver, USA, June 2-10, 2017, Oral presentation.
2. I. Yeboah, G. Fan K. R. Rout, Jia Yang, and D. Chen, *Catalytic in situ co/pyrolysis of biomass powder and heavy fraction of bio-oil using Py-GC/MS*, NKS symposium, Oslo Norway, November 6-7,2017, Oral presentation.

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

Post.doc: 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. 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.

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.

Publications and presentations in 2017:

1. D. Peña, L.S. Jensen, A. Cognigni, R. Myrstad, T. Neumayer, W. van Beek, M. Rønning, The effect of copper loading on iron carbide formation and surface species in iron-based Fischer-Tropsch synthesis catalysts, *ChemCatChem. (2018), DOI: 10.1002/cctc.201701673*
2. D. Peña, A. Cognigni, T. Neumayer, W. van Beek, D.S. Jones, M. Quijadad, M. Rønning, Identification of carbon species on iron-based catalysts during Fischer-Tropsch synthesis, *Appl. Catal. A, 554(2018), 10-23*
3. M. Rønning, *In situ characterisation of catalysts without compromising process conditions,* Keynote lecture, ESRF User Meeting 2017, February 6-8 2017, Grenoble, France
4. M. Rønning, *Combining in situ characterization techniques to reveal real-time deactivation mechanisms in Fischer-Tropsch synthesis catalysts,* 253rd ACS National Meeting, April 2-6, 2017, San Francisco, USA

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

Enhanced visible light adsorption TiO_2 based catalysts for photocatalytic H_2 production

Ph.D. Candidate: Muhammad Zubair
Supervisor: Prof. Jia Yang
Co-Supervisor: Prof. Magnus Rønning

To overcome the energy and environment related issues, renewable, clean and carbon-neutral alternative energy sources are urgently needed. Solar energy is the most abundant form of energy among the different renewable energy sources. One of the promising ways is using hydrogen as an energy carrier in order to store solar energy in the form of the chemical bond between two atoms of hydrogen. The stored energy in the form of a hydrogen molecule can then react with oxygen to form water and energy. Water can be split into hydrogen and oxygen by photocatalytic process by utilizing sunlight, a free energy source and zero addition of additional energy consumption and environmental devaluation. Although the study of the photocatalytic water splitting started earlier, however, the efficiency is much far from state-of -the-art performance and practical application and needs dynamic and energetic efforts to overcome the issues of performance, productivity, stability.

Titanium dioxide (TiO2) is n-type ideal semiconductor photocatalysts, which is being widelyused in H2 production, environmental purification, self-cleaning, CO2 reduction, organic synthesis and solar cells due to high thermal stability, cost-effective, nontoxic and environmentally friendly. Due to the wide band gap (3.2 eV) of TiO2, it can only absorb UV light up to 380 nm, which is an intrinsic limitation for the TiO2-based photocatalysts to efficient light harvesting. The charge separation efficiency is a crucial factor for the efficient photocatalytic activity of TiO2. In spite of its versatility, the mobility of electrons in TiO2 is low which affects the electron transport rate leading to a decrease in the collection efficiency of the photogenerated electrons. Numerous TiO2 based photocatalysts have developed for half photocatalytic reaction for H2 by using the sacrificial reagents by utilizing the photogenerated electrons in the conduction band. These inorganic sacrificial reagents can be easily oxidized to produce different harmful products by the photogenerated holes and promote the H2 production reaction and making the photocatalytic system expensive. Till the time, there is no such catalysts available with a stat of the art efficiency, selectivity and stability along with the efficient and ideal photoreduction setup.

In this project, to overcome the above-mentioned problem, various approaches like heterojunction formation of TiO2 with narrow band gap semiconductor, doping of heteroatom, application of co-catalysts will be applied to increase the photocatalytic activity of semiconductor materials (TiO2) which are thermally stable, abundance, cost effective and biocompatibility.

Financial support:
The project is funded by the Faculty of Natural Sciences, NTNU. Norway.

SINTEF projects

Hydrotreating

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

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

Client: Statoil 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 Scientis 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 (Kinetics and Catalysis), John Walmsley and Ingeborg Helene Svenum (Materials physics).

Liquefaction of biomass by fast pyrolysis leads to a bio-oil comprising oxygenated and reactive sugar-derived as well as lignin-derived components. Hydrotreatment of such liquids is attractive both for stabilization (storage) and chemical conversion (transportation fuels, or co-feed). R&D focused initially on full oxygen removal (HDO) at high temperatures (300 – 375 ^{o}C) and H_2 pressures, which is energy (and hydrogen) demanding. An attractive alternative is milder treatment (conditioning/stabilization) to partially deoxygenated products, with an oxygen content optionally allowing for co-processing in existing refineries. Alternative non-noble metal containing nano-scale catalysts are aimed at to efficiently hydrogenate such oils. Mild HT has been addressed in the temperature range 100 – 300°C for model components and mixtures of aldehydes, alcohols, phenolics and carboxylic acids.
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 in 2017:

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, Oral 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 carbide catalysts as an alternative to Mo sulfides*"

6. 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
7. Daria Otyuskaya, Rune Lødeng, Joris W. Thybaut, Guy B. Marin, "Anisole hydrotreatment Kinetics on CoMo catalyst in the Absence of Sulfur: experimental investigation and model construction", Energy & Fuels 31 (7) 2017 7082 - 7092 (DOI: 10.1021.acs.energyfuels.7b00519)
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 MoO3 and carburized analogues", Biomass Conversion and Biorefinery, Springer 7 (2017) 343 - 359 (DOI 10.1007/s13399-017-0252-z)
9. Chanakya Ranga, Rune Lødeng, Vaios I. Alexiadis, Tapas Rajkhowa, Hilde Bjørkan, Svatopluk Chytil, Ingeborg H. Svenum, John Walmsley, Joris Thybaut, "Effect of composition and preparation of supported MoO3 catalysts for anisole hydrodeoxygenation, Chem. Eng. Journal, 335 (2018) 120 – 132 (https://doi.org/10.1016/j.cej.2017.10.090)

Upgraded scenarios for intergration of biofuel value chains into refinery processes (4Refinery, 2017 – 2021)

Project category: Horizon 2020, "Development of next generation biofuel technologies"; SINTEF is project coordinator (Duncan Akporiaye)

Staff SINTEF (WP3, co-HT and co-HDO, Repsol lead): Senior Scientist Rune Lødeng, Research Scientist Håkon Bergem and Research Scientist Roman Tschentscher.

4REFINERY will develop and demonstrate the production of next generation biofuels from more efficient primary liquefaction routes (Fast pyrolysis and Hydrothermal liquefaction) integrated with upgraded downstream (hydro)refining processes (FCC and HT) to achieve overall carbon yields of >45%. The consortium will aim for successful deployment into existing refineries, including delivering a comprehensive toolbox for interfacing with existing refinery models.

The main objectives of 4REFINERY are:
- To develop new biofuels production technology while at the same time increase understanding and control of the entire value chain
- To scale up materials and testing procedures to define scenarios for the best further implementation in existing refineries
- To develop solutions to answer key societal & environmental challenges

The project will focus on the transformation of bio-liquids from fast pyrolysis and hydrothermal liquefaction into advanced biofuels, through intermediate process steps combined with downstream co-processes technologies. The goal will be to bring these technologies from TRL3-4 to TRL4-5. The project will establish relations between product's properties, the quality of renewable feedstocks and all relevant process parameters along the value chain. The study of these combinations will allow a full understanding of the influence of feedstock and treatment processes on product characteristics.

4REFINERY will (i) use cheap biomass, (ii) require low capital costs processes at small scale, (iii) reduce costs for further treatment due to scaling up and reduction in OPEX and (iv) leverage with existing infrastructure, ensuring the new developments can be rapidly implemented at a commercial scale for production of biofuel with lowest prices compared to its alternatives.

An R&D base for reduced exhaust emissions in the Norwegian maritime transportation sector (EmX 2025, 2015 – 2019)

Project category: Researcher project from the Research council of Norway. Project lead, NTNU, Prof. Hilde J. Venvik.

Staff (SINTEF): 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 environmental friendly marine propulsion. With LNG as fuel it is critical that methane emissions (slip) are controlled to very low levels since methane is a greenhouse gas with more than 20 times the global warming potential than CO_2. The proposed project targets new knowledge and innovation for emissions abatement, more specifically nitrogen oxides (NO_x) and methane (CH_4) in the marine sector. It is a collaboration project between NTNU and SINTEF. NTNU is focused on selective catalytic reduction and SINTEF is focusing on methane abatement for natural gas engines in the marine sector. Success criteria are to obtain > 90% methane conversion below 500 ºC in excess of oxygen, presence of H_2O and CO_2, and possibly also potential poisons like NO_x, NH_3, SO_x and S (from fuel, lubricant or added as odorant). Highly active and stable catalysts based on transition metal oxides are under development. Noble metals are included in the study as reference materials.

Client: The Research Council of Norway TRANSPORT 2025 Program through contract no. 246862. An advisory board with industrial stakeholders (SINTEF Ocean, Gasnor, Bergen Engine AS, Yara) has been established.

Publications

1. Jia Yang, Rune Lødeng, Hilde Venvik, Catalytic methane oxidation for emission control, Oral presentation (Jia) at 9th ICED, Newcastle, Australia (10 – 13. July, 2016)
2. Jia Yang, Rune Lødeng, Hilde Venvik, Co and Ni spinel catalysts for low temperature methane total oxidation, Poster P3.279 Europacat 2017, 29 – 31 August, Florence Italy
3. Jia Yang, Ragnhild Lund Johansen, Rune Lødeng, Hilde J. Venvik, Co and Ni spinel catalysts for low temperature methane total oxidation, Poster iCSI/NKS meeting, Hurdalssjøen 6. – 7. november 2017

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.

Process Development of Moving Bed Carbonate Looping Phase I and II

At present the key team is:
Fjell Technology Group (FTG, the owner of the project): Torleif Madsen (Administrative Management), Dr. Asbjørn Strand (Project Management and R&D Specialist), Jonny Vassdal (Mechanical Design Specialist), Leif Gunnar Madsen (CEO, Commercialisation)
NTNU: Prof. De Chen, Prof.Edd A. Blekkan, Dr.Li He.
SINTEF: Dr.Kumar R Rout

The moving bed carbonate looping concept (MBCL) has been developed by NTNU/SINTEF/FTG since 2017. In CLIMIT project MBCL phase I, the concept of heat integration to calciner is done by catalytic combustion, where modified dolomite sorbent is considered and process efficiency is calculated using ASPEN. It is found that the energy efficiency of NGCC power plant with PCCC is 55.9% points, whereas the NGCC plant without CO2 capture is 57.6% point, as reported by MBCL phase I Q1-Q2 report. An innovative moving bed reactor (MBR) is proposed in the MBCL phase I and is reported in our filed MBCL patent II. In the MBR, one or more mass transfer regions are arranged such that, the solid reactant is retained within the one or more mass transfer regions as the solid reactant flows through the mass transfer system and the mass transfer between the gas and the solid reactant occurs in the one or more mass transfer regions.

The doped dolomite sorbent is tested for ca 200 carbonation and calcination cycles using dry condition and the sorbent possess excellent chemical stability (MBCL Phase I Q2-Q3 report).

However, in the real flue gas from the NGCC power plant contains water vapour; thus it is essential to study the doped dolomite powders in the wet condition. Efforts has been made to study the doped dolomite capture behaviour in the wet condition and the sorbent powder possess excellent capture capacity (above 0.1 gCO2/g-sorbent) and stability for ca 50 carbonation and calcination cycle (MBCL Phase I Q2-Q3 report), which is best reported data yet. A new, one step procedure to combine materials doping and palletisation is developed to simplify the process, thus decrease pellet production cost.

Apart from this a proper kinetic study needs to be done in order to develop kinetic model, which will be implemented MBCL hot (numeric) reactor model that will be developed in the phase II. Cold flow MBCL reactor consists of multi-channel carbonator, calciner MBR and riser will be built in the proposed MBCL phase II, equal to the hot rig design The cold flow integrated reactor is an important step in the reactor scaling up to the validation of the fluid dynamics for both gas and solid in the reactors. In addition, the project will focus also design of the sealing section between two reactors. Based on the cold flow results, the whole system including the cyclones and loop seals will be added to the MBCL (hot) numeric MBCL circulation. In the MBCL technology, heat is provided to endothermic calciner from catalytic combustor through a molten salt heating and cooling loop. In the phase II, the proper selection of molten salts, and experimental demonstration and optimization of the integrated system of catalytic combustion- and calciner-molten salts loops will be carried out. Heat transfer coefficient from solid bed to molten salt tube will be determined by combined experimental work and CFD analysis, which is the important parameter in a proper MBCL plant design for the phase III. At the end of the phase II, the PCCC process with MBCL technology will be simulated by combining fluid dynamics and kinetics of carbonation- and calcination- and total combustion processes. The project will provide a numeric operation of the whole MBCL hot reactor system, which is combination of the MBR, the riser and the tubular reactor for total combustion, will be utilized for building MBCL pilot unit in the phase III.

Financial Support:

The MBCL project is financially supported by GASSNOVA

Philosophiae Doctor (PhD) theses in 2017

Marthe Emelie Melandsø Buan: *Nitrogen-doped Carbon Nanofibers for the Oxygen Reduction Reaction.* NTNU 2017:78

Ida Hjort; *Catalysis for electrochemical conversion of CO2 in aqueous solutions.* Doctorial theses at NTNU, 2017:82

Marie Døvre Strømsheim; *Co{11-20} and Pd3Au{100} single crystals as catalyst model system.* Doctorial theses at NTNU, 2017:372

Disputas Marthe Buan: 29.03.17. From left: Prof. Hilde Venvik, Prof. Magnus Rønning, Marthe Buan, Prof. Bastian J. M. Etzold, Dr. Alejandro Oyarce Barnett

Rector Gunnar Bovim and Dr. Marthe Buan together at the Doctoral Awards Ceremony

Disputas Ida Hjort: 31.03.17. From left: Prof. De Chen, Prof. Petra de Jongh, Ida Hjort, Prof. Gabriele Centi, Assoc. Prof. Størker Moe

Disputas Marie Strømsheim: 13.12.17. From left: Prof. Hilde Venvik, Marie Strømsheim, Prof. Anne Borg, Prof. Karoliina Honkala, Dr. Kees-Jan Weststrate

Master (Diploma) Students in 2017

Ragnhild Brokstad Lund-Johansen; *Catalytic conversion of biomass derived oxygenates to aviation fuel*

Stine Hansen; *Catalytic conversion of biomass derived oxygenates to aviation fuel*

Jianyu Ma; *Metal Dusting*

Björn Frederik Baumgarten; *One-pot conversion of biomass to chemicals on Ni-Cu-Zn alloy catalysts*

Moses Mawanga; *CO_2 Capture using CaO-based (doped and synthetic) sorbents.*

Daniel Skodvin; *Synthesis and applications of carbon spheres*

Petter Kaalstad; *One-pot conversion of cellulose to 5-hydroxymethylfurfural*

Sebastian Langfjæran; *Synthesis and characterization of Tungsten Carbide*

Exchange Bachelor Students in 2017

Nicolas Beck, Germany; *Oxidation of methanol to formaldehyde over Ag catalyst*

Maleki Bakali-Henou, France*; Catalytic combustion of methane on nickel cobalt based catalysts derived from hydrotalcite precursors*

Matus Bodnar, Slovakia*; Direct Non-Oxidative Conversion of Methane to C2 Hydrocarbons, Aromatics and Hydrogen*

Exchange and Master Students in 2017

2016-2017 Master students at NTNU (from left to right): Moses Mawanga, Jianyu Ma, exchange Master student Leyman Maleki Bakali-Hemou (France), Ragnhild Lund-Johansen, Sebastian Langfjæran, Stine Hansen, Daniel Skodvin, Signe Marit Hyrve, Björn Frederik Baumgarten, Petter Kaalstad. Photo: Estelle Vanhaecke, NTNU

Group meetings with seminars

Spring 2017

Location: K5-428/429

Schedule	Time	Presenter	Topic
January 13	14:00	Hilde Venvik for Jia Yang	Methane oxidation for emission control
January 27	14:00	Cornelis Gerardus van der Wijst	Selective catalytic conversion of cellulose to platform chemicals
February 10	14:00	Eleni Patanou	The impact of sequential H_2-COH_2 activation treatment on the structure and performance of Co based catalysts for the Fischer-Tropsch Synthesis.
February 24	14:00	Wenyao Chen	Engineering Pt/carbon composites towards highly efficie nt catalysts for hydrogen production from ammonia borane hydrolysi s
March 10	14:00	Xiaoyang Guo	Investigation of Metal Dusting Corrosion Process over Incoloy 800
March 24	14:00	Seminar for John Walmsley	State-of-the-art catalyst characterization by TEM and related techniques
May 5	14:00	Issac Yeboah	A Tandem C-C reactions of model Aqueous Fraction of Bio-Oil to transport Fuel Precursor``
May 19	14:00	Endre Fenes	Rational Design of $CuCl_2$ /Al_2O_3 based Oxychlorination Catalysts
June 13	14:00	Jaako Alto	DFT simulations of heterogeneous catalysts on bimetallic clusters and substrate effects.

Autumn 2017

Location: K5-428/429

Schedule	Time	Presenter	Topic
August 25	14:00	Shirley E. Liland	Unprecedented Active and Stable Ni-Co Bimetallic Catalyst for Steam Methane Reforming: Combined DFT, Microkinetic Analysis and Kinetic Study.
September 8	14:00	Qingjun Chen	CO activation mechanism of FTS on hcp Co studied by density functional theory using K adsorption as a probe.
September 22	14:00	Katarzyna Swirk	Novel hydrotalcite-derived catalysts for dry reforming of methane.
October 6	14:00	Jørgen Svendby	Carbon-Supported Ru@Pt Core Shell Catalyst for Direct-Methanol Fuel Cell: Interpretation of Measurements of Potential of Zero Total Charge on the Potential-Determining Step
October 20	14:00	Ljubisa Gavrilovic	Influence of potassium species on Co based Fischer-Tropsch catalyst - An experimental and theoretical study
November 6-7		iCSI seminar + Norsk katalysemøte	
November 17	14:00	Mari Helene Farstad	CO oxidation over Pd-based alloys
December 13	14:00	Karolina Honkala	Selectivity in heterogeneous catalysis from first principles
December 15	14:00	Magnus Rønning	Stanford Chronicles
December 18	14:00	Julelunsj	

Courses given by Group Members

TKP4110 Chemical Reaction Engineering

Coordinator: Professor Edd A. Blekkan

Lecturers: Professor Edd A. Blekkan,
Assoc. Prof Jia Yang,
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

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 2017

1. Baidoo, Martina Francisca; Fenes, Endre; Rout, Kumar Ranjan; Fuglerud, Terje; Chen, De, *On the effects of K and La co-promotion on $CuCl_2/\gamma$-Al_2O_3 catalysts for the oxychlorination of ethylene*, *Catalysis Today*, 2017, 299, 164-171

2. Bergem, Håkon; Xu, Run; Brown, Robert C.; Huber, George W., *Low temperature aqueous phase hydrogenation of the light oxygenate fraction of bio-oil over supported ruthenium catalysts*, *Green Chemistry*, 2017, 19, 14, 3252-3262

3. Buan, Marthe Emelie Melandsø; Muthuswamy, Navaneethan; Walmsley, John; Chen, De; Rønning, Magnus, *Nitrogen-doped Carbon Nanofibers for the Oxygen Reduction Reaction: Importance of the Iron Growth Catalyst Phase*, *ChemCatChem*, 2017, 9, 1663-1674

4. Cao, Yueqiang; Sui, Zhijun; Zhu, Yian; Zhou, Xinggui; Chen, De, *Selective Hydrogenation of Acetylene over Pd-In/Al2O3 Catalyst: Promotional Effect of Indium and Composition-Dependent Performance*, *ACS Catalysis*, 2017, 7, 7835-7846

5. Chen, Qingjun; Svenum, Ingeborg-Helene; Qi, Yanying; Gavrilovic, Ljubisa; Chen, De; Holmen, Anders; Blekkan, Edd Anders, *Potassium adsorption behavior on hcp cobalt as model systems for the Fischer–Tropsch synthesis: a density functional theory study*, *Physical Chemistry, Chemical Physics – PCCP*, 2017, 19, 12246-12254

6. Chen, Wenyao; Li, Dali; Peng, Chong; Qian, Gang; Duan, Xuezhi; Chen, De; Zhou, Xinggui, *Mechanistic and kinetic insights into the Pt-Ru synergy during hydrogen generation from ammonia borane over PtRu/CNT nanocatalysts*, *Journal of Catalysis*, 2017, 356, 186-196

7. Chen, Wenyao; Li, Dali; Wang, Zijun; Qian, Gang; Sui, Zhijun; Duan, Xuezhi; Zhou, Xinggui; Yeboah, Isaac; Chen, De, *Reaction mechanism and kinetics for hydrolytic dehydrogenation of ammonia borane on a Pt/CNT catalyst*, *AIChE Journal*, 2017, 63, 60-65

8. Chytil, Svatopluk; Kure, Milly; Lødeng, Rune; Blekkan, Edd Anders, *Performance of Mn-based H_2S sorbents in dry, reducing atmosphere – Manganese oxide support effects*, *Fuel*, 2017, 196, 124-133

9. Dadgar, Farbod; Myrstad, Rune; Pfeifer, Peter; Holmen, Anders; Venvik, Hilde Johnsen, *Catalyst Deactivation During One-Step Dimethyl Ether Synthesis from Synthesis Gas*, *Catalysis Letters*, 2017, 147, 865-879

10. Feng, Xiang; Sheng, Nan; Liu, Yibin; Chen, Xiaobo; Chen, De; Yang, Chaohe; Zhou, Xinggui, *Simultaneously Enhanced Stability and Selectivity for Propene Epoxidation with H_2 and O_2 on Au Catalysts Supported on Nano-Crystalline Mesoporous TS-1*, *ACS Catalysis*, 2017, 7, 2668-2675

11. Gao, Biaofeng; Zhou, Haitao; Chen, De; Yang, Jianhong, *Porous carbon with small mesoporesas an ultra-high capacity adsorption medium*, *Applied Surface Science*, 2017, 420, 535-541

12. Guo, Xiaoyang; Gunawardana, Daham; Chen, De; Vanhaecke, Estelle Marie M.; Venvik, Hilde Johnsen; Walmsley, John**,** *Investigation of metal dusting corrosion process over UNS N08800 alloy*, *NACE International*, 2017, ISBN 978-1-5108-40348, 12 s.

13. Guo, Xiaoyang; Panditha Vidana, Daham Sanjaya Gunawardana; Chen, De; Vanhaecke, Estelle Marie M.; Venvik, Hilde Johnsen; Walmsley, John, *Investigation of metal dusting corrosion process over UNS N08800 alloy*, *International Corrosion Conference Series*, 2017, 4, 2802-2813

14. Lillebø, Andreas Helland; Rytter, Erling; Blekkan, Edd Anders; Holmen, Anders, *Fischer–Tropsch Synthesis at High Conversions on Al_2O_3-Supported Co Catalysts with Different H_2/CO Levels*, *Industrial & Engineering Chemistry Research*, 2017, 56, 13281-13286

15. Lødeng, Rune; Bergem, Håkon, *Stabilization of pyrolysis oils. I: Direct thermochemical liquefaction for energy applications*, Woodhead Publishing Limited, 2017, ISBN 978-0-08-101029-7, 193-247

16. Lögdberg, Sara; Yang, Jia; Lualdi, Matteo; Walmsley, John; Järås, Sven; Boutonnet, Magali; Blekkan, Edd Anders; Rytter, Erling; Holmen, Anders, *Further insights into methane and higher hydrocarbons formation over cobalt-based catalysts with γ-Al_2O_3, α-Al_2O_3 and TiO_2 as support materials*, *Journal of Catalysis*, 2017, 352, 515-531

17. Mahmoodinia, Mehdi; Åstrand, Per-Olof; Chen, De, *Tuning the Electronic Properties of Single-Atom Pt Catalysts by Functionalization of the Carbon Support Material*, *Journal of Physical Chemistry C*, 2017, 121, 20802-20812

18. Qi, Yanying; Ledesma Rodriguez, Cristian; Yang, Jia; Duan, Xuezhi; Zhu, Yi-An; Holmen, Anders; Chen, De*, Adsorption energy-driven carbon number-dependent olefin to paraffin ratio in cobalt-catalyzed Fischer-Tropsch synthesis*, *Journal of Catalysis*, 2017, 349, 110-117

19. Rout, Kumar Ranjan; Baidoo, Martina Francisca; Fenes, Endre; Zhu, Jun; Fuglerud, Terje; Chen, De, *Understanding of potassium promoter effects on oxychlorination of ethylene by operando spatial-time resolved UV–vis–NIR spectrometry*, *Journal of Catalysis*, 2017, 352, 218-228

20. Rytter, Erling; Holmen, Anders, *Perspectives on the Effect of Water in Cobalt Fischer-Tropsch Synthesis*, *ACS Catalysis,* 2017, 7, 5321-5328

21. Sandell, Anders; Schaefer, Andreas; Ragazzon, Davide; Farstad, Mari Helene; Borg, Anne, *Adsorption and photolysis of trimethyl acetate on TiO_2(B)(001) studied with synchrotron radiation core level photoelectron spectroscopy*, *Surface Science,* 2017, 666, 104-112

22. Sevault, Alexis; Khalil, Roger Antoine; Enger, Bjørn Christian; Skreiberg, Øyvind; Goile, Franziska; Wang, Liang; Seljeskog, Morten; Kempegowda, Rajesh Shivanahalli*, Performance Evaluation of a Modern Wood Stove Using Charcoa*l, *Energy Procedia*, 2017, 142, 192-197

23. Strømsheim, Marie Døvre; Knudsen, Jan; Farstad, Mari Helene; Sørvik, Linn Cecilie; Guo, Xiaoyang; Venvik, Hilde Johnsen; Borg, Anne, *Near Ambient Pressure XPS Investigation of CO Oxidation Over Pd3Au(100)*, *Topics in catalysis*, 2017, 60, 1439-1448

24. Tsakoumis, Nikolaos; Walmsley, John; Rønning, Magnus; van Beek, Wouter; Rytter, Erling; Holmen, Anders, *Evaluation of Reoxidation Thresholds for γ-Al_2O_3-Supported Cobalt Catalysts under Fischer - Tropsch Synthesis Conditions*, *Journal of the American Chemical Society*, 2017, 139, 3706-3715

25. Venvik, Hilde Johnsen; Yang, Jia, *Catalysis in microstructured reactors - Short review on smallscale syngas production and further conversion into methanol, DME and Fischer-Tropsch products*, *Catalysis Today*, 2017, 285, 135-146

26. Wang, Di; Ji, Jian; Chen, Bingxu; Chen, Wenyao; Qian, Gang; Duan, Xuezhi; Zhou, Xinggui; Holmen, Anders; Chen, De; Walmsley, John, *Novel Fe/MnK-CNTs nanocomposites as catalysts for direct production of lower olefins from syngas*, *AIChE Journal*, 2017, 63, 154-161

27. Wang, Hongmin; Blaylock, D. Wayne; Dam, Anh Hoang; Liland, Shirley Elisabeth; Rout, Kumar Ranjan; Zhu, Yi-An; Green, William H.; Holmen, Anders; Chen, De, *Steam methane reforming on a Ni-based bimetallic catalyst: Density functional theory and experimental studies of the catalytic consequence of surface alloying of Ni with Ag*, *Catalysis science & technology*, 2017, 7, 1713-1725

28. Wang, Xuehang; Li, Yahao; Lou, Fengliu; Buan, Marthe Emelie Melandsø; Sheridan, Edel; Chen, De, *Enhancing capacitance of supercapacitor with both organic electrolyte and ionic liquid electrolyte on a biomass-derived carbon*, *RSC Advances*, 2017, 7, 23859-23865

29. Yanying Qi, Christian Aaserud, Jia Yang, Anders Holmen, De Chen: Mechanistic insights into the size dependent water effect on selectivity in Fischer_Tropsch on Co catalysts. J. Catal. (2017) Accepted

30. Erling Rytter, Anders Holmen: Perspectives on the Effect of Water in Cobalt Fischer-Tropsch Synthesis , ACS Catalysis 7 (2017) 5321-5328

Presentations in 2017

1. Guo, Xiaoyang; Gunawardana, Daham; Chen, De; Vanhaecke, Estelle Marie M.; Venvik, Hilde Johnsen; Walmsley, John, *Investigation of Metal Dusting Corrosion Process over UNS N08800 Alloy*, NACE CORROSION 2017, March 26-30, New Orleans, Louisiana, USA (RCN project, GASSMAKS)

2. Rønning, Magnus, *Combining in situ characterization techniques to reveal real-time deactivation mechanisms in Fischer-Tropsch synthesis catalysts*, 253rd American Chemical Society National Meeting, April 2-6, San Francisco, California, USA

3. Van der Wijst, Cornelis; Duan, XueZhi; Liland, Ingvild Skeie; Siri F., Morken; Rui, Haakon Marius Vatten; Walmsley, John C.; Zhu, Jun; Wang, Aiqin; Zhang, Tao; Chen, De, *Diols from cellulose in a one pot reaction: Tuning the selectivity on Nickel Zinc alloys*, International Symposium on Green Chemistry, 2017, May 13-16, La Rochelle, France

4. Fenes, Endre; Baidoo, Martina Francisca; Rout, Kumar Ranjan; Fuglerud, Terje; Chen, De, *Rational Design of CuCl2/Al2O3 based Oxychlorination Catalysts*, NAM25 | North American Catalysis Society Meeting, 2017, June 4-9, Denver, USA

5. Liland, Shirley Elisabeth; Wang, Yalan; Qi, Yanying; Rout, Kumar Ranjan; Chen, De, *Unprecedented Active and Stable Ni-Co Bimetallic Catalyst for Steam Methane Reforming: Combined DFT, Microkinetic Analysis and Kinetic Study*, NAM25 | North American Catalysis Society Meeting, 2017, June 4-9, Denver, USA (RCN project, GASSMAKS)

6. Sevault, Alexis; Khalil, Roger Antoine; Enger, Bjørn Christian; Skreiberg, Øyvind; Goile, Franziska; Wang, Liang; Seljeskog, Morten; Kempegowda, Rajesh Shivanahalli, *Performance evaluation of a modern wood stove when using charcoal*, 25th European Biomass Conference & Exhibition, 2017, June 12-15, Stockholm, Sweden

7. Chen, De; Mahmoodinia, Mehdi; Astrand, Per Olof, *Frontiers in carbon nanomaterials for energy conversion: from 0 to 3 dimensions*, International Symposium on Carbon Research Frontiers, 2017, June 22, Sydney, Australia

8. Li, Yahao; Chen, De, *Fe/N/P tridoped biomass derived carbon electrocatalyst for highly efficient ORR*, Carbon 2017, June 23-28, Melbourne, Australia (NTNU project)

9. Sevault, Alexis; Khalil, Roger Antoine; Enger, Bjørn Christian; Skreiberg, Øyvind; Goile, Franziska; Wang, Liang; Seljeskog, Morten; Kempegowda, Rajesh Shivanahalli, *Performance Evaluation of a Modern Wood Stove Using Charcoal*, 9th International Conference on Applied Energy, 2017, August 21-24, Cardiff, UK

10. Buan, Marthe Emelie Melandsø; Muthuswamy, Navaneethan; Walmsley, John; Chen, De; Rønning, Magnus, *Nitrogen-doped carbon nanofibers for oxygen reduction: The role of iron in forming active ORR sites*, Europacat, 2017, August 27-31, Florence, Italy (EU project, FREECATS)

11. Farstad, Mari Helene; Strømsheim, Marie Døvre; Knudsen, Jan; Fernandes, Vasco Rafael; Borg, Anne; Venvik, Hilde Johnsen, *CO oxidation over Pd-based alloys*, Europacat, 2017, August 27-31, Florence, Italy (NTNU project)

12. Yang, Jia; Johansen, Ragnhild Lund; Lødeng, Rune; Venvik, Hilde Johnsen, *Co and Ni spinel catalysts for low temperature methane total oxidation*, Europacat 2017, August 27-31, Florence, Italy

13. Guo, Xiaoyang; Vanhaecke, Estelle Marie M.; Ma, Jianyu; Gunawardana, Daham; Walmsley, John; Chen, De; Venvik, Hilde Johnsen, *Investigation of initial stage of Metal Dusting Corrosion Process over Inconel 601*, EUROCORR2017 20th International Corrosion Congress & Process Safety Congress 2017, September 3-7, Prague, Czech Republic (RCN project, GASSMAKS)

14. Guo, Xiaoyang; Gunawardana, Daham; Vanhaecke, Estelle Marie M.; Chen, De; Venvik, Hilde Johnsen; Walmsley, John, *Characterization of metal dusting corrosion on instrumentation used in natural gas conversion technologies*, Nordic Nanolab User Meeting, 2017, September 9-10, NTNU, Trondheim, Norway (RCN project, GASSMAKS)

15. Medvedovski, Eugene; Ma, Jianyu; Guo, Xiaoyang; Vanhaecke, Estelle Marie M.; Venvik, Hilde Johnsen, *Studies of Corrosion Resistance of Aluminized Coatings in Metal Dusting Environments*, Materials Science & Technology, 2017, October 8-12, Pittsburgh, PA, USA (RCN project, GASSMAKS)

16. Farstad, Mari Helene; Strømsheim, Marie Døvre; Knudsen, Jan; Fernandes, Vasco Rafael P; Borg, Anne; Venvik, Hilde Johnsen, *CO oxidation over Pd-based alloys, Norwegian catalysis symposium,* 2017, November 6-7, Hurdal, Norway (NTNU project)

17. Liland, Shirley Elisabeth; Rout, Kumar Ranjan; Fenes, Endre; Yang, Jia; Chen, De, *Rational Design of Ni-Co/Hydrotalcite Catalyst for Methane Total Combustion using operando UV-Vis spectroscopy*, Norwegian Catalysis Symposium 2017, November 6-7, Hurdal, Norway (RCN project, GASSMAKS)

18. Yang, Jia; Lund Johansen, Ragnhild; Lødeng, Rune; Venvik, Hilde Johnsen, *Catalytic abatement of CH4 slip*, Norwegian catalysis symposium, 2017, November 6-7, Hurdal, Norway

19. Lødeng, Rune; Yang, Jia; Lervold, Stine; Bingen, K.; Venvik, Hilde Johnsen, *Global models for predicting methanol to formaldehyde (MTF) performance*, ICSI seminar, November 6-7, Hurdal, Norway

20. Anders Holmen* & Erling Rytter: Fischer-Tropsch Synthesis on Cobalt Catalysts – On the Effect of Water. Invited Lecture, 253rd ACS National Meeting, April 2-6 2017 San Francisco, USA

21. L. Gavrilovic*, J. Brandin, A. Holmen, H.J. Venvik, R. Myrstad, E.A. Blekkan: Lecture. Deactivation of Co-based Fischer-Tropsch catalyst by aerosol deposition of potassium salts. Norwegian Catalysis Symposium, Hurdalsjøen Hotel, November 6th and 7th 2017.

22. Y. Wang*, L. Xao, Y. Qi, Y. Zhu, J. Yang, D. Chen, A. Holmen: Microkinetic analysis of light olefins production from synthesis gas: Combined UBI-QEP method and BEP relationship. Poster. Norwegian Catalysis Symposium, Hurdalsjøen Hotel, November 6th and 7th 2017.

23. J. Yang, Z. Yu, Ø. Borg, A. Holmen, D. Chen: Insights on effects of carbon support and Co particle size on the C_{5+} selectivity of Fischer-Tropsch synthesis. Poster (P3.258). 13th EuropaCat. 27-31 August, 2017, Florence, Italy.

24. Y. Wang*, L. Xiao, Y. Qi, S.E. Liland, K.R. Rout, Y.-A. Zhu, J. Yang, D. Chen, A. Holmen: Micokinetic analysis of steam methane reforming over transition metal surfaces, combined DFT calculations and UBI-QEP method. Lecture. 13th EuropaCat. 27-31 August, 2017, Florence, Italy.

25. Q. Chen*, I.-H. Svenum, Y. Qi, L. Gavrilovic, D. Chen, A. Holmen, E.A. Blekkan: CO activation mechanism of Fischer-Tropsch synthesis on hcp Co studied by density functional (DFT) using K adsorption as a probe. Lecture. 13th EuropaCat, 27-31 August, 2017, Florence, Italy.

26. Gavrilović, E.A. Blekkan, H.J. Venvik, A. Holmen, R. Myrstad and J. Brandin: Influence of Potassium species on Cobalt Based Fischer-Tropsch Catalyst Using Aerosol Deposition Technique Poster (P-M-BRM-26). North American Catalysis Society Meeting, June 4-9, 2017, Denver, Co, USA.

Popular science contributions

1. Rønning, Magnus; "A catalyst for discussion." ESRF News, March 15, 2017

Seminars 2017

-Recycling Energy-

Cambi & Technology Development

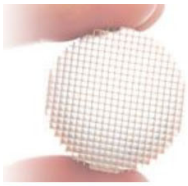
Presentation at Department of Chemical Engineering
by Pål Jahre Nilsen, Andreas Helland Lillebø and Anne-Lise Hjelseth

Tuesday January 17 at 1215 in K5-428

Cambi is the leading provider of technology for conversion of organic waste streams to renewable energy and high-quality bio fertilizer. The company was originally founded in 1989. Today Cambi has more than 130 employees and is represented in more than 11 different countries. Since 1995 we have built 47 plants with a further 10 plants under construction. These plants have the capacity to treat sludge and food waste from more than 50 million people in 21 different countries. Find out more at http://www.cambi.com/.

The presentation will focus on how Cambi contributes to important technology development today as well as future technology development needs. We would like to explore future R&D cooperation opportunities with relevant institutes at NTNU. Cambi's trainee program and competence requirements will also be described, including the relevance of PhD training.

The presentation is open to everyone interested, but especially relevant to students and employees at the Department of Chemical Engineering (IKP). The Cambi representatives will be available for discussions after the presentation. Coffee and a small snack will be provided.



iCSI

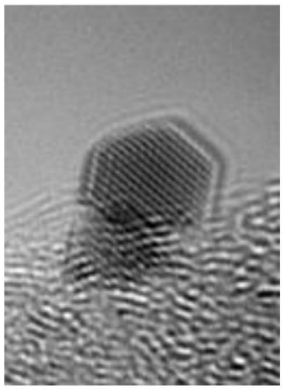
sfi = Centre for Research-based Innovation

NTNU – Trondheim Norwegian University of Science and Technology

KinCat
Catalysis Group – SINTEF – NTNU

Seminar, Friday March 24 2017 10:00 to 14:00 in the iCSI room KV 428-29

State-of-the art catalyst characterization by transmission electron microscopy (TEM) and related techniques



The KinCat group (NTNU-SINTEF Gemini Centre) has long collaborated with the Department of Physics, NTNU, and SINTEF Materials and Chemistry on catalyst characterization by transmission electron microscopy and related techniques. The efforts have resulted in new insight and expansion of the characterization toolbox to new instrumentation at NTNU as well as elsewhere. At the core of this collaboration has worked Dr. John C. Walmsley, Senior Scientist at SINTEF MK and Adjunct Professor at NTNU. In relation to John's transfer to Cambridge University as Senior Technical Officer, we found it appropriate to summarize some of the achievements and discuss future opportunities for collaboration. The seminar is open to all students and staff at KinCat and the TEM Gemini Centres.

Light lunch will be served to those registering by Wed 22 March to Estelle Vanhaecke: estelle.m.vanhaecke@ntnu.no

Tentative program:

1030-1040	Hilde Venvik	Opening
1040-1105	Anders Holmen	*Pt-Re(Sn) and Co-Re catalysts studied by TEM*
1105-1130	Erling Rytter	*Imaging in development of commercial Fischer-Tropsch catalysts*
1130-1150	Hilde Venvik	*Microstructured reactors/catalysts and metal dusting*
1155-1245		LUNCH
1250-1330	John Walmsley	*Future opportunities for electron microscopy in catalysis – overview and discussion*

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-408, 13:15, March 30, 2017

13:15 **Catalysis for solar driven chemistry: opportunities and challenges**

Prof. Gabriele Centi, University of Messina, Italy

iCSI annual meeting and Norwegian Catalysis Symposium 2017

Monday the 6th

08:00	*Departure from Hurdalsjøen Hotel to Hamar and K.A. Rasmussen*
09:15	*Arrival and check in at K.A. Rasmussen*
09:20	*Company's introduction and plant tour*
10:45	*Departure for Hurdalsjøen Hotel*
11:00	iCSI / NKS registration opens
12:00	Lunch
13:00	iCSI welcome
13:10	**IIA1**: Prof. Anja Sjålstad (UiO) *"21st century Ammonia Oxidation and Nitric Acid technology development"*
13:30	**IIA2**: Dr. Karl Isak Skau (YARA) *"New NOx abatement technologies for the marine market and state-of-the-art SCR catalysis"*
13:50	**IIA3**: Dr. Jasmina Hafizovic Cavka (SINTEF) *"Frontier formalin technology development"*
14:10	**IIA4**: Dr. Kumar R. Rout (SINTEF) *"PVC Value Chain: World class energy and raw material efficiency for the production of Chlorine and Vinyl Chloride Monomer (VCM)"*
14:30	**IIA5**: Prof. Stian Svelle (UiO) *"The next step in direct activation of lower alkanes"*
14:50	**IIA6**: Prof. Magnus Rønning (NTNU) *"Generic projects for additional industrial synergies"*
15:10	Coffee break
16:50	NKS welcome
17:00	**Plenary Lecture**: Prof. Enrique Iglesia (University of California, Berkeley) **"Towards More Accurate Descriptions of Reactivity in Acid and Oxidation Catalysis on Metal Oxides"**
18:00	Poster session (Common for iCSI and NKS)
19:30	Dinner

Tuesday the 7th

8:30	**Plenary Lecture:** Prof. Graham Hutchings (Cardiff Catalysis Institute) ***"Catalysis using gold"***		
9:30	Coffee break		
9:50	iCSI - IIA1: **Ata ul Rauf Salman** (NTNU) "Catalysts for Attaining NO-NO2 Equilibrium"	9:50	NKS: **Carlos A. Grande** (SINTEF) Additive manufacturing as a tool to reshape catalytic reactors
10:05	iCSI - IIA2: **Silje Fosse-Håkonsen** (SINTEF) "TBA"	10:10	NKS: **Kun Guo** (UiS) Unravelling the Size Effect of Monodispersed Nickel Nanoparticles in the Hydrolysis of Ammonia Borane
10:20	iCSI - IIA3: **Stine Lervold** (NTNU) "TBA"	10:30	NKS: **Isaac Yeboah** (NTNU) Insight into catalytic in-situ co/pyrolysis of biomass powder and heavy fraction of bio-oil using Py-GC/MS
10:35	iCSI - IIA4: **Endre Fenes** (NTNU) "TBA"	10:50	NKS: **Sondre Eliasson** (UiB) The Mechanism of Rh-catalyzed Transformation of Fatty Acids to Linear Alpha-Olefins; a DFT-Study
10:50	iCSI - IIA5: **Michael Dyballa** (UiO) "TBA"	11:10	NKS: **Ingeborg-Helene Svenum** (SINTEF) Co(11-20) as a model system for investigating adsorption, surface restructuring and poisoning effects in Fischer-Tropsch chemistry
11:05	iCSI - IIA6: **Samuel Regli** (NTNU) "*In situ* characterization of iCSI catalysts by DRIFTS, Raman, X-ray spectroscopy and diffraction"	11:30	NKS: **Mari Helene Farstad** (NTNU) CO oxidation over Pd-based alloys
11:20	iCSI - IIA6: **Annett Thøgersen** (SINTEF) "TBA"	11:50	NKS: **Irene Pinilla-Herrero** (UiO) Dehydrogenation vs hydrogen transfer activity of Zn-ZSM-5 catalytic systems in methanol conversion to aromatics
11:35	iCSI - IIA6: **Oleksii Ivashenko** (UiO) "*Reactor STM for Catalysis*"		
12:00	Lunch		
13:00	**Plenary Lecture**: Prof. Alessandra Beretta (Polytecnico di Milano) ***"New challenges in the SCR technology for stationary applications: a focus on Hg oxidation"***		
14:00	Coffee break		
14:20 - 16:20	**iCSI** Board meeting (*for only board members and SAC*)	14:20	NKS: **Sigurd Øien-Ødegaard** (UiO) ***NKS award lecture for best PhD thesis*** Preparation, structure, and reactivity of functionalized zirconium metal-organic frameworks
		15:00	NKS: **Ljubiša Gavrilović** (NTNU) Deactivation of Co-based Fischer-Tropsch catalyst by aerosol deposition of potassium salts
		15:20	NKS: **Marco Foscato** (UiB) Loss and Reformation of Ruthenium Alkylidene: Connecting Olefin Metathesis, Catalyst Deactivation, Regeneration, and Isomerization
		15:40	NKS: **Dimitrios K. Pappas** (UiO) Searching for the Active Sites Responsible for the CH_4 to CH_3OH Conversion over Cu-Chabazite Materials
		16:00	NKS: **Shirley E. Liland** (NTNU) Rational Design of Ni-Co/Hydrotalcite Catalyst for Methane Total Combustion using operando UV-Vis spectroscopy
		16:20 - 16:30	NKS closing

Dear KinCat colleagues,

It is a pleasure to invite you for a short seminar in connection to Marie's defense, offered by the two external committee members:
Time: Dec 13 at 13:00-15:00
Place: iCSI and KinCat rooms, i.e. K5.429 and K5.428

Karoliina Honkala, Professor of Computational Nanocatalysis, Nanoscience Center, Department of Chemistry, University of Jyväskylä, Finland:
Selectivity in heterogeneous catalysis from first principles

Kees-Jan Weststrate, Senior Research Scientist. Dutch Institute for Fundamental Energy Research (DIFFER), The Netherlands:
Surface Science investigations of the Fischer-Tropsch reaction on Cobalt

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

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

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

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 Nanoparticles 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*

Marthe Emelie Melandsø Buan: *Photoelectrochemical CO_2 Reduction to Alcohols. 2017*

Ida Hjort*: State of the art and perspectives in catalytic processes for CO_2 conversion into chemicals and fuels. 2017*

Marie Døvre Strømsheim: Metal-Organic-Frameworks (MOFs) – Properties and applications in catalysis. 2017

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: December 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: Toolbox Systems AS

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: 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 Trondheim

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
Defense 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 Muthuswamy
Platinum based Catalysts for Methanol Fuel Cells: Metal Clusters and Carbon Supports.
Defense of thesis: December 2011
Current positions: Post. doc. Aalto University, Finland

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
Curren position: Franzefoss Minerals, Hylla

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: Beyonder AS, Stavanger

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 spectroscopy 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
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Current position: Post.doc. Department of Materials Science and Engineering and A. J. Drexel Nanomaterials Institute, Drexel University, Philadelphia , PA 19104 USA

Marthe Emelie Melandsø Buan
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Defense of thesis: March 29 2017
Current position: Post. doc. Aalto University, Finland

Ida Hjort
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Current position: NAMMO Raufoss

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