Annual Report

2015

KinCat

Catalysis Group – SINTEF – NTNU

KinCat
Strong Point Centre Kinetics and Catalysis

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

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Annual Report 2015
KINCAT
Strong Point Centre Kinetics and Catalysis

Contents

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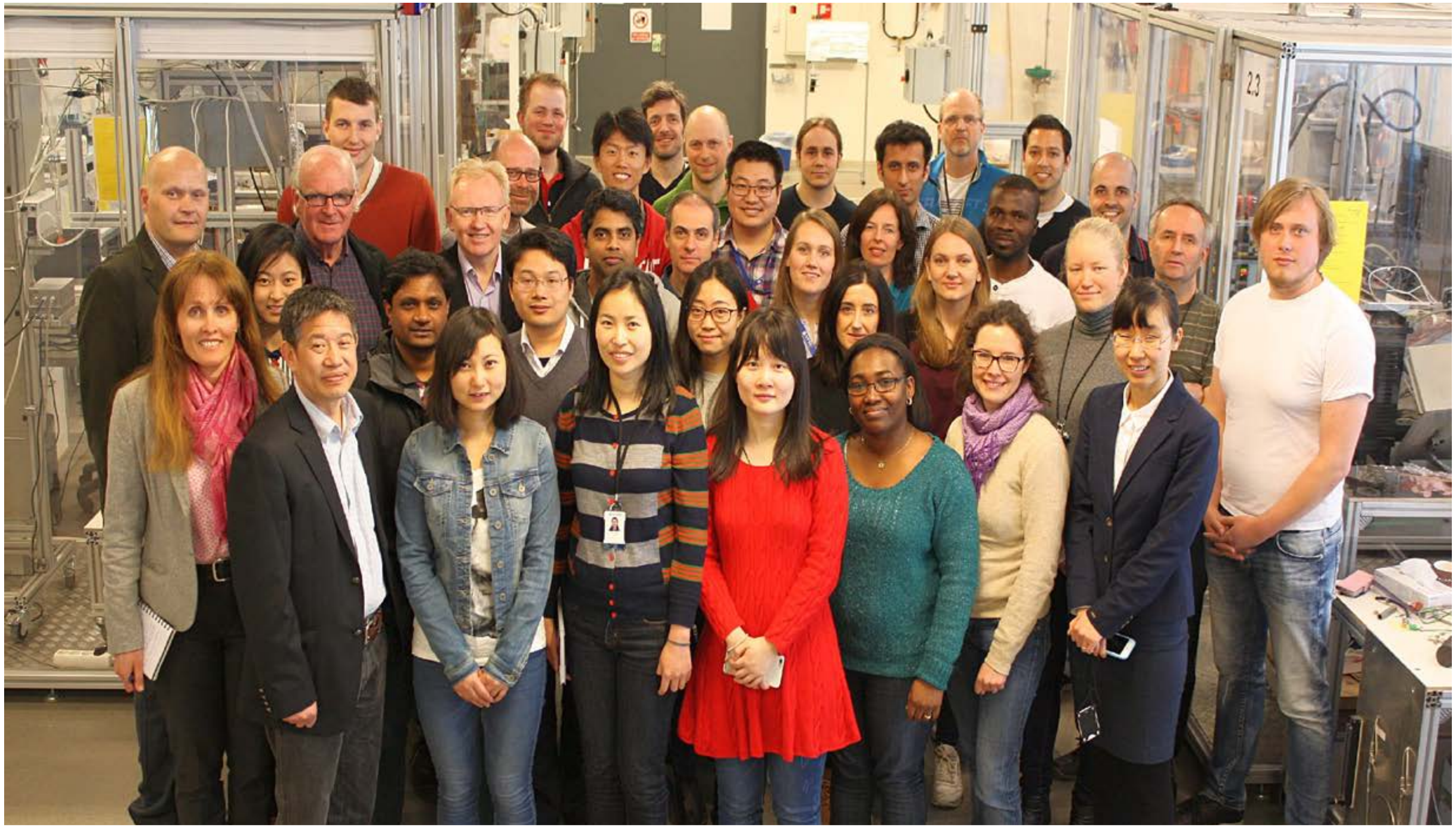


Fourth row: Ljubisa Gavrilovic, Håkon Bergem, Endre Fenes, Xiaoyang Guo, Torbjørm Gjervan, Bjørn Christian Enger, Yahao Li, Eirik Pedersen, Ata Salman, Rune Myrstad, Diego Alexander Pena Zapata
Third row: Magnus Rønning, Di Wang, Anders Holmen, Edd Anders Blekkan, Kumar Rajan Rout, Andrea Cognigni, Karin Wiggen Dragsten, Camilla Otterlei, Shirley Elisabeth Liland, Isaac Yeboah, Cristian Ledesma Rodriguez, Rune Lødeng
Second row: Hilde Venvik, Daham Gunawardana Sanjaya Vidana, Qingjun Chen, Cui Ting, Victoria Gil Matellanes, Mari Helene Farstad, Cornelis van der Wijst
First row: De Chen, Yalan Wang, Jia Yang, Xuehang Wang, Martina Francisca Baidoo, Estelle Vanhaecke, Yanying Qi
Not present: Charitha Udani, Eleni Patanou, Erling Rytter, Farbod Dadgar, Haakon Rui, Hilde Bjørkan, Ida Hjort, Ingeborg- Helene Svenum, Kuiyi You, Marie Døvre Strømsheim, Marthe Emelie Buan, Michael Marcus Wycisk, Nikolaos Tsakoumis, Svatopluk Chytil, Xavier Auvray

Research Areas

❖ Conversion of Natural Gas

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

❖ Upgrading of Oil Fractions

- Hydrotreating
- Catalytic reforming/isomerization

❖ 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 liquification

❖ High Temperature Chemistry

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

❖ Environmental Catalysis

- Sulfur reduction by hydrotreating
- Preferential oxidation of CO
- Wastewater treatment
- CO_2 conversion

❖ Fundamental Studies of Heterogeneous Catalysis

- Surface science
- Preparation of catalytic materials (supported metals and metal oxides, zeolites, supports, nanoparticles)
- Kinetics (steady-state and transient kinetics, SSITKA)

- Adsorption and diffusion in porous media
- Catalyst deactivation (sintering, coke formation)
- Characterization of heterogeneous catalysts
- Reactor, kinetic and first principles (DFT) modeling

❖ Microstructured Reactors and Membrane Reactors

❖ Production and Application of Carbon Nanomaterials, Carbon Nanofibers, Nanotubes and Graphene

❖ Photocatalysis

- Water splitting.
- Photoreforming

Main Laboratory Equipment

❖ Reaction Laboratories

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

❖ Catalyst Preparation Laboratory

- Spray drier
- Ball mills
- Furnaces

❖ Catalyst Characterization

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

Highlights from the Activities in 2015

- Two candidates completed their PhD degrees in 2015. Andrey Volynkin and Anh Hoang Dam. The titles of the dissertations and pictures of the candidates/committees/supervisors are enclosed.

- 18 Master students completed their thesis in 2015. Their name and titles are enclosed.

- iCSI – industrial Catalysis Science and Innovation – is the new 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. In 2015 the contract was established, the first PhD and postdoctoral fellows were recruited, and several research activities started. A description of iCSI is enclosed.

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

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

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

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

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

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

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

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

Centre for Research-based Innovation
The Research Council of Norway

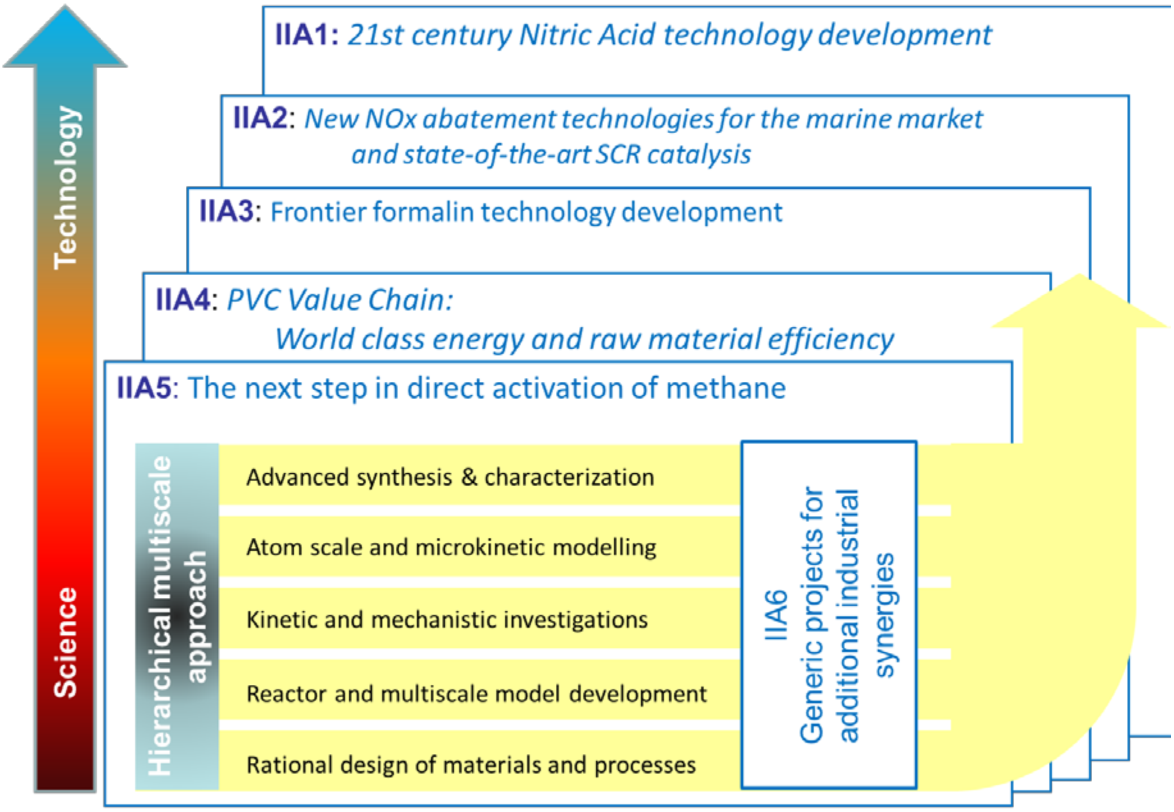
iCSI is a Centre for research based innovation (SFI) granted 2015-23by the Research Council of Norway, with the industrial partners Yara, K.A. Rasmussen, Dynea, Inovyn and Haldor Topsøe AS and the research partners University of Oslo (UiO), SINTEF and Norwegian University of Science and Technology (NTNU). NTNU is host institution with Prof. Hilde J Venvik as Centre Director.

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 (IIAs, see bottom figure), through:

- 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.

In 2015, the Contract with the Research Council of Norway was established, including a Consortium Agreement between the partners involved. The Work Plan for the first 4 years was laid out, and the first research activities were started. Several PhD and postdoctoral fellowships were recruited to the Centre, as well as the Centre Coordinator Estelle Vanhaecke. The iCSI 2015 Annual Report is available through the new iCSI website:

https://www.ntnu.edu/icsi



Ph.D. Candidates and Postdoctoral Projects

Microwave-assisted preparation and thermal aging of Pt/Al_2O_3 catalyst

Postdoctoral fellow: Xavier Auvray
Supervisors: Professor Magnus Rønning, Professor Edd A. Blekkan

Utilization of conventional ovens to evaporate the solvent after incipient wetness impregnation is common in catalyst preparation. However, the heating of the catalyst particles by surrounding hot air is heterogeneous and slow, which affects the metal particle distribution inside the pores as well as their size. As microwaves interact directly with polar molecules such as water, more homogeneous heating of the impregnated support could be ensured. In addition microwave heating is able to quickly transfer energy to the material and thereby considerably decrease the drying time. Small and homogeneously dispersed metal particles can therefore be expected from this method.

Pt/Al_2O_3 catalyst will be prepared by conventional and microwave-assisted methods and compared. The effect of further microwave irradiation on the particle size and NO oxidation activity will be studied and compared to convective thermal aging.

Financial support: NTNU, Department of Chemical Engineering.

Nitrogen-doped Carbon Nanofibers on Expanded Graphite as Oxygen Reduction Electrocatalysts

Ph.D. candidate: Marthe Emelie Melandsø Buan
Supervisor: Prof. Magnus Rønning
Co-supervisors: 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 metals currently used. However, in acidic conditions the ORR-activity and stability still remain lower than that of Pt. 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 N-doped carbon nanofibers

(N-CNFs) is performed and the possible active sites are explored by correlating the catalyst performance with the “physico¨ chemical properties.

A catalytic CVD method is employed to grown nitrogen-doped carbon nanofibers on expanded graphite from Fe and Ni particles 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, TEM and EELS is performed to correlate the N-CNF properties with the oxygen reduction activity. The active sites for the oxygen reduction are further explored by post-treatment of the N-CNFs with HNO_3 and KOH.

Publications and presentations in 2015:

1. M.E.M. Buan, N. Muthuswamy, J.C. Walmsley, D. Chen, M. Rønning, *Nitrogen-doped Carbon Nanofibers on Expanded Graphite as Oxygen Reduction Electrocatalysts,* Carbon, 101 (2016) 191–202.
2. Navaneethan Muthuswamy, Marthe E. M. Buan, De Chen, Magnus Rønning, *Engineering of Nitrogen-doped Carbon Nanofibers for the ORR by Chemical Vapor Deposition*, Oral presentation, ECS conference on Electrochemical Energy Conversion and Storage with SOFC - XIV, Glasgow, Scotland, 30. July 2015.
3. Marthe E. M. Buan, Navaneethan Muthuswamy, John C. Walmsley, De Chen, Magnus Rønning, *Engineering of N-CNFs on Exfoliated Graphite for the Oxygen Reduction Reaction,* Poster presentation, Electrolysis and Fuel Cell Discussions 2015, La Grande Motte, France, 13-14. September 2015.

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

Fundamental studies on the role of potassium in cobalt-based FTS catalysts

Post. Doc: Qingjun Chen
Supervisor: Professor Edd A. Blekkan

Cobalt-based Fischer-Tropsch synthesis (FTS) catalysts, which have high activity, stability and low CO_2 selectivity, are promising to be used in the biomass to liquids (BTL) processes. For the syngas produced from biomass, trace impurities such as potassium (K) and sodium (Na) are usually detected. It has been demonstrated that very low concentrations (below 100 ppm alkaline metal) could result in a significant decrease of the FTS activity and alter the selectivity to hydrocarbons while it has almost no effect on the cobalt dispersion, the H_2/CO chemisorption amount and heat of adsorption of H_2 or CO. It seems difficult to elucidate the role of trace amounts of K in the reaction mechanism of FTS just based on the experimental work. In this project, density functional theory (DFT) calculations are employed to investigate the role of potassium in cobalt-based FTS catalysts.

Initially, K adsorption behavior on the hcp cobalt was studied using DFT calculations. The surface energy calculation and Wulff construction of the equilibrium shape of hcp cobalt identified 9 facets that can be exposed. K adsorption on the 9 exposed facets indicated that the terrace facet (0001) and step/step-like facets (10-11) and (10-12) were the most preferred facets for adsorption, with the highest adsorption energy of about -2.4 eV. The corrugated facets (11-20), (11-21), (11-24) and (21-30) exhibited lower K adsorption energies (-2.08~-2.31 eV), and would not be preferred for adsorption. Furthermore, it was found that the adsorption energy was significantly influenced by coverage. This was probably due to strong repulsive interaction between adsorbed K atoms. The diffusion energy barrier calculation results indicated that K atoms are mobile on terrace facets (0001) with a very low barrier of 0.01 eV. On stepped facets, the K diffusion from one step to another is difficult due to a high barrier of 0.44~ 0.55 eV, however, on the terrace of the same step K is mobile. The role of K in CO adsorption and activation in Fischer-Tropsch synthesis was systematically studied. DFT investigations of the coadsorption of CO-K and H-K on typical terrace (0001) and step (10-12) facets showed that K significantly improved CO adsorption on hcp Co but slightly inhibited the adsorption of H_2.

<u>Presentations in 2015:</u>

1. Qingjun Chen, Ingeborg-Helene Svenum, Yanying Qi, Ljubisa Gavrilovic, De Chen, Anders Holmen, Edd A. Blekkan, *Potassium adsorption behaviors on hcp cobalt: A density functional theory calculation*, the11th Natural Gas Conversion Symposium, Tromsø, Norway, 5-9 June,2016.
2. Qingjun Chen, Ingeborg-Helene Svenum, Yanying Qi, Ljubisa Gavrilovic, De Chen, Anders Holmen, Edd A. Blekkan, *Potassium adsorption behavior and its influence on the CO adsorption and activation on hcp cobalt in Fischer-Tropsch synthesis*, the 16th International Congress on Catalysis, Beijing, China, 3-8 July, 2016.

Financial Support: This project is financed by the ENERGIX programme in the Norwegian Research Council.

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

Post. Doc: Andrea Cognigni
Supervisor: Prof. Magnus Rønning

This project aims towards enhanced sensitivity and selectivity by using Modulation Enhanced Spectroscopy (MES) applied to X-ray Absorption Spectroscopy (XAS).

A promising approach for enhancing the surface sensitivity of conventional bulk techniques such as XAFS and XRD is modulation enhanced experiments. The ME technique utilizes an imposed periodic variation of an external parameter (stimulus), such as temperature, pressure, concentration, and light flux, which excites, i.e. alters and influences, the species of interest, thus adding selectivity to measurements. The resulting periodically varying response can be selectively detected and the signal-to-noise ratio can be significantly enhanced by the phase sensitive detection (PSD) method of the ME technique, where the time-domain periodic response is converted to the corresponding phase-domain response. The ME technique has shown unique strength when combined with broadband analytical methods such as IR and Raman spectroscopy, allowing kinetic differentiation of various responses residing within a spectrum and hence giving insights into transformation mechanisms and pathways. A new approach in software application to the XAS data is realized. Efforts are aimed at extracting pure components from the overall XAS signal using multivariate curve resolution (MCR). MCR has been applied to a series of XAS data sets in order to separate individual components from the total signal.

The approach has been successfully applied to a number of experiments at the Swiss Norwegian beamline (SNBL) using a Pt-based catalyst. Absorption and desorption of CO from the Pt surface of the catalyst have been modulated. Application of MCR to the dataset has allowed us to isolate the adsorption of CO. This highlights the power of MCR in the detection of weak spectral contributions arising from surface interactions. The project is a collaboration with the Swiss-Norwegian Beamlines (SNBL), France and the Institute of Chemical Research of Catalonia (ICIQ), Spain.

Poster presentations:

1. Cognigni, N. E. Tsakoumis, W.van Beek, A. Urakawa, M. Rønning, *Multivariate Component Resolution (MCR) applied on X-ray Absorption spectroscopy. A suitable technique for processing large datasets*, 5th International Conference on Operando Spectroscopy - Deauville (france) - May 17, 2015 – May 21, 2015
2. Cognigni, N. E. Tsakoumis, W.van Beek, A. Urakawa, M. Rønning, *Multivariate Component Resolution (MCR) applied on X-ray Absorption spectroscopy. A suitable technique for processing large datasets,* XAFS16 - 23 -28 August 2015, Karlsruhe (Germany)

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

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

PhD-candidate: Farbod Dadgar
Supervisors: Prof. Hilde J. Venvik, Prof. Anders Holmen, Senior Scientist Rune Myrstad

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

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

Publications and presentations in 2015:

1. Farbod Dadgar, Rune Myrstad, Peter Pfeifer, Anders Holmen, Hilde J. Venvik. *Direct dimethyl ether synthesis from synthesis gas: The influence of methanol dehydration on methanol synthesis reaction*. Catalysis Today 270 (2016) 76-84.
2. Farbod Dadgar, Rune Myrstad, Peter Pfeifer, Anders Holmen, Hilde J. Venvik. *Direct Dimethyl Ether Synthesis from Synthesis Gas:the Influence of Methanol Dehydration on Methanol Synthesis Reaction*. EuropaCat XII; Aug.30 – Sept.04, Kazan, Russia. Oral presentation.

Financial support:

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

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.

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

While both promoters are able to displace copper from the support surface vacancies, increasing the amount of active $CuCl_2$ supported on the catalyst. However, after the initial increase, potassium forms a mixed chloride salt with copper, inhibiting ethylene adsorption and/or Cl migration, decreasing the number of active sites and inhibiting the reaction. Thus, the less active K promoted catalysts might be used in the initial part of an industrial reactor, limiting hotspot formation due to the exothermic reactions, while the more active Ce promoted catalyst could be allocated towards the reactor outlet thus keeping a more uniform temperature distribution throughout the reactor.

Financial support: This project is funded by iCSI.

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

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

The essence of this project is to better understand alkali effects on Co-based Fischer-Tropsch catalyst, an issue relevant to the conversion of biomass to liquid fuels via gasification. Biomass contains a wide range of inorganic and organic species, some of which can act as catalyst poisons. Potassium is a key element in this respect, present in the form of volatile species (typicaly salts such as KCl, K_2SO_4, $K_2CO_3$and KOH) after gasification. Previous work shows that even small amounts of alkali species can result in severe deactivation of Co catalysts.

Standard Fischer-Tropsch catalyst (20%Co/0.5%Re/γAl_2O3) was exposed to the 4 different potassium salts (KCl, K_2SO_4, K_2CO_3 and KNO_3) using an aerosol deposition technique. With this technique it is possible to simulate the actual process in the BTL plant, where the alkali species will be transported in the gas phase. Catalysts poisoned by KNO_3 were calcined in air and after calcination the potassium is expected to be present as K_2O on the catalyst. Results from characterization techniques, such as elemental analysis, H_2 chemisorption, BET surface area, TPR, together with the results from the Fischer Tropsch synthesis i.e. CO conversion, selectivity, and activity will be compared with the same catalyst without any poison and also with previous results where the alkali was deposited using incipient wetness impregnation.
Project name: Advanced Biofuels via Synthesis Gas

Financial support: The Research council of Norway, ENERGIX (contract no: 10417501) programme.
Collaboration: Linnaeus University, Växjø, Sweden

Presentations in 2015:

1. Ljubiša Gavrilović, Edd A. Blekkan, Anders Holmen, Hilde J. Venvik, Jan Brandin, *Fischer-Tropsch Synthesis – investigation of Co catalyst by exposure to aerosol particles of potassium salts.* The 15th Norwegian Catalysis Symposium, Bergen, Norway, 2015.

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

Ph.D. Candidate: Xiaoyang Guo
Supervisor: Professor Hilde Johnsen Venvik
Co-supervisor: Professor De Chen and Senior Scientist John Walmsley

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

In this study, we are focusing on understanding the metal dusting mechanism and identifying possible controlling variables in view of compact technology for generation and conversion of syngas. Alloy samples relevant to micro-reactors (Incoloy 800 series) were tested in the experimental setup under metal dusting conditions. Carefully polished and ultrasonically cleaned alloy coupons were first oxidized at temperatures in 500–1000ºC range to generate oxide layers of varying structures and composition. The oxidized samples were then exposed to different carburizing gas atmospheres (either 10%CO/Ar or simulated syngas compositions) for varying time-on-stream (1-20 h), pressure (1-20 bar) and temperature (550,650 and 750 ˚C). Samples before and after the carbonaceous gases exposure were investigated by means of optical microscopy, scanning/transmission electron microscopy (SEM/TEM), Auger electron spectroscopy (AES) and Raman spectroscopy. Surface carbon deposits were also studied by TEM equipped with an energy-dispersive X-ray spectrometry (EDS). Finally, the results of Incoloy 800 will be compared with those of Inconel 601 from another project.

The amount of carbon formed on Incoloy 800 is clearly a function of exposure temperature and time as well the gas composition. The alloy samples treated under CO+Ar at low temperature and low pressure (i.e. 550 ˚C and 1 bar) showed a thick layer of surface carbon deposits. The amount of carbon formed on the surface decreases, however, with the exposure temperature and this requires further investigation in view of the infinite carbon activity and presumed kinetic control under such conditions. Existence of carbon formation could so far not be confirmed under the syngas mixture, irrespective of the exposure temperature and pressure, and this is in partial contrast to our previous investigations of Inconel 601. Bulk composition analysis confirms that the Incoloy 800 contains more Fe and less Ni compared to Inconel 601, while the Cr content in both alloys is more or less the same. Since the compositions of the two alloys are different, Incoloy 800 will likely form a different surface oxide layer under oxidation pre-treatment, and its characteristics and initial performance under carbonaceous gases will be addressed and compared to existing results. Further characterization of selected short exposure samples will enable a better link between the surface structure and composition, and the initiation of the carbon formation.

Financial support:

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

Aqueous electrochemical CO_2 reduction on CuZnOCNT catalysts

PhD Candidate: Ida Hjorth
Supervisor: Prof. De Chen

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

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

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

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

Posters/Presentations:

1. I. Hjorth, S. F. Morken, N. Muthuswamy, D. Chen, *Electroreduction of CO_2 on CNT-supported copper and copper-zinc alloys*, International Solar Fuels Consortium, April 2015, Uppsala, Sweden
2. I. Hjorth, N. Muthuswamy, D. Chen, *Effects from modifying carbon nanofiber supports on metal nanoparticle catalyzed CO_2 reduction*, ISE, October 2015, Taipei, Taiwan

Graphene synthesis and application

Ph.D. candidate: Yahao Li
Supervisor: De Chen

For decades, fuel cell and metal-air battery attract huge amount of attentions as the need for clean and renewable energy never ends. And as the key components of above devices, catalysts for oxygen reduction reaction (ORR) are intensively investigated. Platinum (Pt) base catalysts, including Pt alloy, are by far the most efficient among all catalysts. However, as one of the noble metal, the lack of abundance of Pt lead to the high cost, which hinders its commercial applications. Recent studies revealed that heteroatoms (N, B, S or P) doped carbon nanomaterials possess impressive ORR activities and co-doping of the heteroatoms (normally N with a second heteroatom) can further enhances the ORR activity. This makes doped carbon nanomaterials wonderful alternatives to Pt for ORR.

We used a simple method to utilize the electrochemical exfoliated graphene (EEG) and biomass derived carbon to produce N & P co-doped graphene (NPG) and applied them in ORR as the electrocatalyst. The produced NPG samples from both carbon sources have specific surface area (SSA) higher than 2000 m^2/g. The ORR activity was tested using rotating disk electrode and the LSV data shows that the over potential and the half-current potential of NPG are almost the same as commercial Pt/C. Since the active site of nitrogen doped graphene is the carbon atoms with Lewis basicity next to pyridinic N, we believe that when co-doped with P, the chance to produce carbon atoms with Lewis basicity is increased, and with the high SSA of NPG, the exposure chance of the active sites also increased. As a result, the ORR activity of NPG is comparable to Pt/C, which makes it a wonderful ORR catalyst.

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

Kinetic Study of Bimetallic Catalysts for Compact Steam Reformer

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

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

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

There are two catalysts needed for this reactor, one for each reaction. For the SR reaction a bimetallic Ni based catalyst supported on a hydrotalcite-like structure will be the main focus. There has already been performed several studies on different catalytic metals for steam reforming, including bimetallic Ni catalysts. However not much attention has been given to the compact reformer, which means there are many aspects of the catalytic compact reformer that still needs to be investigated. The combustion catalysts will be based on Al coated on a calcinated FeCrAl alloy felt, an additional coat of Co-ZrO2 will be applied before Co-MnO2 is deposited by impregnation or Pechini methods. However, also the bimetallic Ni catalyst for the SMR will be tested for the combustion reaction.

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.

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

Integrated *H_2BioOil* process for efficient biofuel production

Postdoctoral Fellowship: Dr. María Victoria Gil Matellanes
Supervisor: Professor De Chen

The aim of this project is to provide experimental proof of an integrated *H_2BioOil* process for fully sustainable production of biofuels from lignocellulosic biomass. The integrated process includes high pressure fast-hydropyrolysis (FHP) of wood biomass powders in hydrogen, followed by an immediate downstream vapor-phase catalytic aldol-condensation (CAC) and catalytic hydrodeoxygenation (HDO) to produce hydrocarbon products (C_4-C_{16+}). The system is also integrated with pressure swing sorption enhanced steam reforming (SESR) of the byproducts from the process to produce hydrogen at high pressure. This is a novel process with a high fuel yield and high energy efficiency, and it represents a fully sustainable process of hydrogen generation from biomass. The global goal of the project is to provide the experimental proof-of-concept for sustainable production of drop-in transportation fuels from biomass.

Fast-hydropyrolysis involves a rapid heating of biomass up to temperatures of about 500 ºC in a high pressure (about 20 bar) hydrogen environment to produce vapors, which sequentially will be catalytically aldol-condensed/ketonizated and hydrodeoxygenated to produce hydrocarbon products (C_4-C_{16+} and C_1-C_3), CO, CO_2, H_2 and H_2O. These products, except C_4-C_{16+}, will be treated by sorption enhanced steam reforming to produce H_2 at high pressure (about 20 bar), which will be integrated in the FHP reactor. In the SESR process, high-temperature CO_2 sorbents are incorporated into the catalyst bed to in situ remove the carbon dioxide from the gaseous phase. Hence, the thermodynamic equilibrium limits of the reversible reforming and water gas shift (WGS) reactions are shifted towards the hydrogen production, so obtaining a high hydrogen conversion in a single step.

The first objective of the project is to build the high pressure fast-hydropyrolysis reactor and study the effect of the temperature on the fast-hydropyrolysis process in order to produce low char yield and low water content in the liquid product. The composition of the products obtained from this process will be measured by liquid-chromatography mass-spectrometry (LC-MS). Subsequently, the high pressure fast-hydropyrolysis reactor will be integrated with CAC, HDO, and SESR reactors.

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

Publications in 2015: (not related to the project)

1. Gil, María Victoria; Fermoso, Javier; Rubiera, Fernando; Chen, De. *H_2 production by sorption enhanced steam reforming of biomass-derived bio-oil in a fluidized bed reactor: An assessment of the effect of operation variables using response surface methodology.* Catalysis Today 2015; Volum 242. s.19-34.

New approach to metal dusting corrosion

Post.doc.: Dr. Daham S. Gunawardana Panditha-Vidana
Supervisor: Prof. Hilde Venvik

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

Surface polished/unpolished coupon-like Ni-based industrial alloy (INCONEL® 601) samples were first subjected to oxidation treatment at different temperatures (540, 760 or 980 ˚C) in gas atmospheres with different steam or oxygen partial pressures (P_{O_2}). Pre-oxidized samples were then exposed to different syngas atmospheres with either *infinite* or *finite* carbon activity ($a_C >> 1$ or $a_C > 1$). The resulting surfaces and carbonaceous products were characterized by means of optical microscopy, electron microscopy (both SEM and TEM) in conjunction with EDS, AES under ion-sputtering and XPS. The TEM results show that formation of filamentous carbon deposits under both *infinite* and *finite* carbon activity conditions has been catalysed by metallic particles containing Ni and Fe.

It is also found that, irrespective of the exposure conditions or the oxidative pre-treatment gas, increasing the pre-oxidation temperature in the range 540–980 ˚C was found to create a surface oxide layer with better resistance to carbon formation. The Ni and Fe content within the surface oxide layer becomes depleted at the higher temperature, allowing formation of a thicker oxide saturated in Cr. Varying the exposure temperature under *finite* carbon activity conditions ($a_C > 1$, 20 bar) produced thick carbon deposits at 650 ˚C and 750 ˚C while little (50% CO) or no (20% CO) carbon was found after the 550 ˚C exposure. Under different CO concentrations (20% or 50%), but constant level of H_2, CO_2 and steam, the amount of carbon formed is clearly a function of exposure temperature and carburizing gas composition. Removal of the carbonaceous deposits from the samples revealed that material degradation had taken place at higher exposure temperatures (either pitting or spallation). Auger depth profile analysis showed that oxidation of the alloy matrix had proceeded alongside the reducing reactions leading to carbon formation under the 20% CO containing gas mixture, while this was not the case under 50% CO.

Presentations and publications in 2015:

1. Gunawardana, P.V.D.S. Hwang, J. Walmsley, J.C. Venvik, H.J. *Catalytic phenomena critical to the initiation of metal dusting corrosion*. Poster presentation at *in*GAP Seminar 2015, Oslo, Norway; March 2-3.
2. Gunawardana, P.V.D.S. Walmsley, J.C. Venvik, H.J. *Study of the initial phase of metal dusting corrosion relevant to natural gas conversion technologies*. Oral presentation at 16th Nordic Corrosion Congress, Stavanger, Norway; May 21.
3. Gunawardana, P.V.D.S. Hwang, J. Walmsley, J.C. Svenum, I.-B. Venvik, H.J. *On the origin and state of Ni and Fe species as catalyst for the initiation of metal dusting corrosion*. Poster presentation at EuropaCat XII, Kazan, Russia; Aug. 30 – Sep. 4.
4. Gunawardana, P.V.D.S. Walmsley, J.C. Venvik, H.J. *Investigation of initial stage of metal dusting corrosion phenomenon relevant to natural gas conversion technologies*. Oral presentation at European Corrosion Congress (EUROCORR), Graz, Austria; Sept 6-10.
5. Gunawardana, P.V.D.S. Walmsley, J.C. Venvik, H.J. *Understanding catalytic phenomena responsible for metal dusting*. Oral presentation at 15th Norwegian Catalysis Symposium, Bergen, Norway; December 4.

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

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

SINTEF: Research Scientist Rune Myrstad and Senior Scientist John Walmsley
NTNU: Postdoc Eleni Patanou, Professor Edd A. Blekkan and Professor Magnus Rønning

Fischer – Tropsch synthesis (FTS) is the heart of Gas-to-Liquids process for the utilization of synthesis gas derived from natural gas. In the Co-based FTS two types of reactors are dominant, the multi-tubular fixed-bed reactor and the slurry bubble-column reactor.

The active phase in FTS is metallic cobalt and the conventional type of catalyst precursors contain an oxide phase that has to go through activation under hydrogen at temperatures exceeding 250 ^{o}C. The use of such catalysts in slurry-phase reactors requires *ex situ* reduction and passivation of the catalyst before it is loaded into the slurry reactor, in order to prevent thermal damage and decomposition of the liquid medium in the slurry. The formation of the metallic cobalt can be alternatively obtained with modification in the synthesis procedure by adding a carburization step performed under CO-rich atmospheres. Subsequently the metal is formed through decomposition of the formed carbide. This occurs under hydrogen at relatively low temperatures (<250 ^{o}C). However the effect of the CO pre-treatment on the catalyst performance remains under debate.

This study focuses on the benefits of CO pre-treatment that can serve as be an alternative activation path done *in situ* in the slurry reactors and at temperatures similar to the actual reaction temperature.

Funding: Statoil R&D and The Research Council of Norway through the GASSMAKS program, NTNU Department of Chemical Engineering.

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

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

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

This project aims at obtaining a better understanding of chain growth and termination in the FTO process as a function of catalyst properties. The work will apply a multiscale approach, integrating first principles calculations (DFT), adsorption microcalorimetry 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 will be investigated by combining experimental and theoretical methods.

The effect of Mn promotion on Co catalysts will be investigated by varying Mn:Co ratios, catalyst preparation method, reaction- and reduction conditions. The state of Mn under relevant reaction conditions will be investigated using *in situ* characterization techniques and the role of Mn in H_2 and CO adsorption on Co will be investigated using adsorption microcalorimetry, TPD and XPS.

The promotion effects of Mn on Co will also be investigated by DFT. Calculations will 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.

Presentations in 2015:

1. Østbye Pedersen, Eirik; Svenum, Ingeborg-Helene; Blekkan, Edd. A. *Co-Mn Catalysts for Fischer-Tropsch Production of Light Olefins.* Oral presentation, 24th North American Catalysis Society Meeting; 14.6.2015-19.6.2015, Pittsburgh, PA, USA.
2. Østbye Pedersen, Eirik; Svenum, Ingeborg-Helene; Blekkan, Edd. A. *Fischer-Tropsch Production of Light Olefins by Mn promoted Co/Al_2O_3 Catalysts.* Oral presentation, 15th Norwegian Catalysis Symposium; 03.12.2015-04.12.2015, Bergen, Norway

Funding: The Norwegian Research Council, contract no. 224968/E30 under the Gassmaks programme.

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

Ph.D. Candidate: Xiaoyang Guo
Supervisor: Professor Hilde Johnsen Venvik
Co-supervisor: Professor De Chen and Senior Scientist John Walmsley

Metal dusting is a corrosive degradation phenomenon on metals and alloys that proceeds by a gradual breakdown of the material into fine particles. It constitutes a problem in the chemical industries, where metals and alloys are extensively exposed to carbon-supersaturated gaseous with low partial pressures of oxygen and/or steam in a critical temperature range of 300–850 ˚C. Metal dusting carries significant cost, since certain precautions need to be taken to avoid catastrophic events in these environments.

Microstructured reactors are being developed for process intensification in order to enable safer, more cost-effective and sustainable conversion of natural gas in the small-to-medium scale. Due to the large inner surface area of the reaction volumes and highly integrated heat exchange between reactant and product streams metal dusting becomes an even more severe issue.

In this study, we are focusing on understanding the metal dusting mechanism and identifying possible controlling variables of metal dusting in the point of compact technology for generation and conversion of syngas. Alloy relevant to micro-reactors (Incoloy 800 series) were tested in the experimental setup under metal dusting conditions. Carefully polished and ultrasonically cleaned alloy coupons were first oxidized at chosen temperatures in 500–1000ºC range for 6 h, under different oxygen partial pressures to generate oxide layers of varying structures and composition. The oxidized samples were then exposed to different carburizing gas atmospheres (either 10%CO/Ar or simulated syngas compositions) for varying time scale from 1 h to 20 h at 1bar to 20bar in the temperature range of 550 ˚C to 750 ˚C. Samples before and after the carbonaceous gases exposure were investigated by means of optical microscopy, scanning electron microscopy (SEM), Auger electron spectroscopy (AES) and Raman spectroscopy. Surface carbon deposits were further studied via transmission electron microscopy (TEM) equipped with an energy-dispersive X-ray spectrometer (EDS). Finally the results of Incoloy 800 will be compared with Inconel 601 which was studied in another project.

Bulk composition analysis shows that the Incoloy 800 contains more Fe and less Ni compared to Inconel 601, while the Cr content in both alloys is more or less the same. Since the compositions of the two alloys are different, Incoloy 800 will likely form a different surface oxide layer under oxidation pre-treatment, and its characteristics and initial performance under carbonaceous gases will be addressed and compared to existing results.

The amount of carbon formed on the sample is clearly a function of exposure temperature and time. Amount of carbon found on the surface of the samples underwent longer carburizing gas exposure is always higher compared to their shorter exposure counterparts. The growing trend of carbon filament on pre-oxidized Inconel 601 samples after CO exposed (10% CO-Ar gas, 650 ˚C, 1bar) for different exposure time. Further characterization of selected short exposure samples will enable a better link between the surface structure and composition, and the initiation of the carbon formation.

The pre-oxidation of Inconel 601 alloy provided samples with an oxide layer on the surface of the alloy enriched in Cr and Al as determined by Auger depth profiling analysis. Samples oxidized at higher pre-treatment temperature form less carbon.

Financial support:
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Mechanism studies of cobalt-catalyzed Fischer-Tropsch synthesis

Ph.D. Candidate: Yanying Qi

Supervisors: Prof. De Chen and Prof. Em. Anders Holmen

Cobalt-catalyzed Fischer-Tropsch (F-T) synthesis, featuring high activity and stability, is a promising option for the conversion of natural gas to transportation fuels. Water, a primary oxygen-containing product in cobalt-catalyzed F-T synthesis, enhances C_{5+} selectivity and olefin/paraffin ratio on most cobalt based catalysts. The understanding of the mechanistic role of water on selectivity is highly desirable for the rational design of F-T catalyst. We studied the underlying nature for the enhancement effect of water on selectivity by using propene hydrogenation as a model reaction. The effect of coadsorbed water, OH and O on adsorption energies and activation energies are evaluated. The DFT calculations demonstrated that the co-adsorbed OH rather than H_2O or O decreases the adsorption of propene and leads to the decrease of TOF. It is therefore suggested that the enhancement of olefin/paraffin ratio with the presence/addition of water in F-T is ascribed to the inhibition of olefin hydrogenation via OH species.

It is crucial to improve the C_{5+} selectivity in F-T synthesis since liquid fuels are of commercial interest. It is commonly accepted that the chain growth takes place by stepwise addition of a monomeric intermediate. In order to provide insights into the understanding of the monomer and the underlying nature of C_{5+} selectivity, all possible C_1+ C_1 coupling reactions has been evaluated. Taking into account the site coverage of the intermediates, the reaction between HCO and CH_2 is suggested to be the most preferred pathway.

Publications and presentations in 2015:

1. Y. Qi, J. Yang, D. Chen, A. Holmen, *Recent Progresses in Understanding of Co-Based Fischer–Tropsch Catalysis by Means of Transient Kinetic Studies and Theoretical Analysis*. Catal. Lett., 145 (2015) 145-161.
2. Y. Qi, J. Yang, D. Chen, A. Holmen, *Mechanistic studies of cobalt-catalyzed Fischer Tropsch synthesis by a combined approach of DFT*

calculations, kinetic isotope effect and kinetic analysis. Poster presentation. 24th North American Catalysis Society Meeting, Pittsburgh, USA. June 14-19, 2015

3. T.H. Pham, Y. Qi, J. Yang, X. Duan, G. Qian, X. Zhou, D. Chen, W. Yuan, *Insights into Hägg Iron-Carbide-Catalyzed Fischer–Tropsch Synthesis: Suppression of CH4 Formation and Enhancement of C–C Coupling on* χ-Fe_5C_2 *(510)*, ACS Catal., 5 (2015) 2203-2208.

Financial support:
The project is funded by Norwegian Research Council through ISP programme.

Catalysts for attaining NO/NO_2 equilibrium

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

Nitric acid is an important industrial chemical. Commercial production of nitric acid takes place via the Ostwald process. The process comprises of three steps [1]

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

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

The reaction is catalyzed by Pt-Rh gauzes. Typical concentrations at the exit of ammonia combustor are NO (10%) and H_2O (15%) [2].

2. Oxidation of the nitric oxide to nitrogen dioxide

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

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

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

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

The objective of the project is to develop an active catalyst to fully oxidize NO to NO_2 in step 2. The catalyst will help to reduce the capital investment by replacing the bulky homogeneous oxidation process by compact heterogeneously catalyzed process. A catalyst working at 300^{o}C has the potential of 15 % additional heat recovery from the NO oxidation process. An experimental set-up for this reaction is currently being designed and constructed. Several potential catalyst systems will be tested. The choice of catalyst will depend upon the activity, selectivity and stability.

The project is a collaboration between Yara, SINTEF and NTNU.

Financial Support: The project is funded by Yara and the Research Council of Norway (NFR) through the iCSI centre.

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

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

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. Co(11-20) represents a model system for cobalt (Co) based Fischer – Tropsch catalysts for conversion of natural gas or biomass into liqiuid fuels. Previous experiments by Lillebø et al. at KinCat found that Co-catalysts with small alkali metal impurity loadings (~N ppm) found that, while the catalytic activity significantly decreased, the H_2 chemisorption properties and the H_2 and CO differential heats of adsorption remained unaffected. Therefore, the deposition of submonolayer amounts of potassium (K) on Co(11-20), and its effect on FTS relevant adsorption phenomena were studied using Low Energy Electron Diffraction (LEED) and Scanning Tunneling Microscopy (STM). Adsorption of CO ($1\text{-}3\times10^{-9}$ mbar) 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 potassium (K), showed notable differences in the reconstruction process and resulted in a surface with a higher degree of disorder in STM. High resolution XPS (HRXPS) at ASTRIDII in Aarhus, Denmark confirmed that K could be removed by standard cleaning cycles between experiments. Further experiments are required, however, to elucidate the effect on K on the adsorption of CO and ethylene.

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 $(\sqrt{5}\times\sqrt{5})R27^\circ$ surface oxide was found to exist on $Pd_3Au(100)$, similar to Pd(100) and $Pd_{75}Ag_{25}(100)$, under oxygen exposure. To further elucidate the effect of Au as an alloying element, CO oxidation over $Pd_3Au(100)$ was studied with Near Ambient Pressure XPS (NAPXPS) and quadropole mass spectroscopy (QMS) at the SPECIES beamline at the MAXIV Laboratory in Lund, Sweden, under oxygen rich conditions (O_2:CO=10:1), and ~1 mbar pressure. QMS data shows 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 O1s 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 $Pd_{75}Ag_{25}(100)$.

Publications and presentations in 2015:

1. M. D. Strømsheim, I.-H. Svenum, A. Borg, H. J. Venvik; *Model Systems for Co Fischer-Tropsch Catalysts,* Poster at NAM24 – 24th North American Catalysis Society Meeting; June 14-19 2015, Pittsburgh, USA.
2. M. D. Strømsheim, I.-H. Svenum, A. Borg, H. J. Venvik; *Model Systems for Co Fischer-Tropsch catalysts.* Poster at EuropaCat XII - 12th European Congress on Catalysis I; Aug. 30 – Sept 4, 2015, Kazan, Russia
3. M. D. Strømsheim, I.-H. Svenum, A. Borg, H. J. Venvik; *Model Systems for Co Fischer-Tropsch catalysts: STM investigations of alkali metal on Co single crystal surfaces.* Oral presentation at ECOSS31 – 31st European Conference on Surface Science; Aug. 31 – Sept 4, 2015, Barcelona, Spain.

Financial support: This project is funded by inGap.

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

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

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

As in any other investigation of catalytic materials, unravelling structure - performance relations is important for the understanding the catalytic processes itself. Co-based FTS is a structure sensitive reaction where the cobalt particle size and phase, in addition to effects from the used support and promotor, are interplay. The high complexity of the reaction dictates that a detailed examination of the catalytic material has to be performed and therefore catalyst characterisation in all the stages of catalyst lifetime is vital.

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

Publications and presentations in 2015:

1. E. Rytter, N.E. Tsakoumis, A. Holmen, *On the selectivity to higher hydrocarbons in Co-based Fischer–Tropsch synthesis*, Catalysis Today (2015) Accepted.
2. N.E. Tsakoumis, A.P.E. York, De Chen, M. Rønning, *Catalyst characterisation techniques and reaction cells operating at realistic conditions; towards acquisition of kinetically relevant information*, Catalysis Science & Technology 5 (2015) 4859-4883.
3. N.E. Tsakoumis, A. Voronov, R. Dehghan, R.E. Johnsen, W. van Beek, P. Norby, J. Walmsley, E. Bergene, S. Eri, Ø. Borg, M. Rønning, E. Rytter, A. Holmen. *In situ monitoring of Co-based Fischer-Tropsch synthesis catalysts*, inGAP- Innovative Natural Gas Processes and Products, closing seminar. Oslo, Norway, 02 – 03 March 2015.

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

Photocatalytic hydrogen production from alcohols

Ph.D. candidate:	Punchi Patabandige Charitha Udani
Supervisor:	Professor Magnus Rønning

Producing hydrogen from photoreforming of hydrocarbons is an emerging field within renewable energy research. Photocatalysts that can operate at ambient temperature without producing harmful by-products are ideal as environmentally sound catalysts. For such systems to be considered in large-scale applications, photocatalytic systems that are able to operate effectively and efficiently in a continuous flow reactor must be established.

The project is mainly focused on producing fuel alternatives with the use of an artificial solar light source (UV and/or visible light) and various photocatalysts. Various hydrocarbons, catalyst synthesis methods and catalysts formulation are used, comparing noble metals with transition metals and combinations of these with the aim to prepare cost-effective catalyst systems.

The project involves synthesis and characterization of nanomaterials with tuneable bandgap, and also testing of the catalyst materials in photocatalytic reactions such as photoreforming of methanol, ethanol and glycerol. The effects of several parameters on the hydrogen production were studied, including metal loading, H2 pre-treatment, light wavelength and alcohol concentration.

Photocatalytic activity measurements are performed in a quartz reactor inside the photoreaction chamber (Luzchem) and monitored with a micro-GC. Complete sets of 14 UVA (350 nm), UVC (254 nm) and visible light (420 nm) lamps are provided with the photoreactor.

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

Publications in 2015:

1. P.P.C. Udani, M. Rønning, *Comparative study on the photocatalytic hydrogen production from methanol over Cu, Pd, Co and Au loaded TiO2*, Oil Gas Sci. Technol. (2015), 70 (5), 831-839

Mesopore-rich Carbon as Supercapacitor Electrode Material with High Energy Density

PhD candidate: Xuehang Wang
Supervisor: Prof. De Chen
Co-supervisor: Dr. Edel Sheridan

There is an increasing need for high power density to keep the stability and sustainability of the grid energy storage, as well as to meet the demand for high-power portable devices. Supercapacitor (SC) is an attractive energy storage option for high power application. However, the moderate energy densities of the SCs limit their wide-spread use.

In the present project work, the high gravimetric capacitance of supercapacitor with good rate capability was achieved by a combine modeling and experimental approach. A large-scalable method was utilized to prepare a series of high-surface area (up to 3400 m^2/g) and mesopores-rich carbon nanosponge (CNS) with varied PSD by tuning carbonization and activation conditions. The prepared materials were tested in carbon-ionic liquid (IL) SCs, and the gravimetric capacitances of SCs were varied from 121 to 290 F/g in neat ionic liquid 1-ethyl-3-methylimidazolium tetrafluoroborate ($EMIMBF_4$) electrolyte. We developed a model of ion packing and demonstrated, quantitively, the significant impact of geometric factor (PSD and ionic size) on the ion-distribution in the pores and hence the gravimetric capacitance. The model predicts satisfactorily the gravimetric capacitance of the CNSs synthesized in our work as well as the reported carbon materials in literatures. The model reveals that the capacitance is determined by the correlation between PSD and an ion-packing function which described the discipline of the ion-distribution in different pore sizes. Based on our model, systematic strategies for rational design of various carbon materials (both micro- and mesoporous and allows broad PSD) and ionic liquids to achieve ultrahigh gravimetric capacitance can be proposed. The mesopore-rich CNS with desired PSD promoted by our model delivered the capacitance up to 290 F/g at 20 ^oC, which is among one of the highest recorded DL capacitance.

Presentation and publications in 2015:

1. Poster presentation: Xuehang Wang, Haitao Zhou, Edel Sheridan, De Chen. ChemEner, Berlin, Germany, Jan, 2015.
2. Poster presentation: Xuehang Wang, Haitao Zhou, Edel Sheridan, De Chen. CESEP2015, Poznan, Poland, Oct, 2015.
3. Oral presentation: Xuehang Wang, Haitao Zhou, Edel Sheridan, De Chen. Nanolab symposium 2015, Trondheim, Norway, Nov, 2015
4. Xuehang Wang, Haitao Zhou, Edel Sheridan, John Charles Walmsley, Dingding Ren, De Chen. *Geometrically-confined favourable ion packing for high gravimetric capacitance in carbon-ionic liquid supercapacitor*. Energy & Environmental Science, 2016, 9: 232-239.
5. Haitao Zhou, Xuehang Wang, Edel Sheridan, De Chen. *Boost the specific energy and cycling stability of dual-manganese oxides-based Li-ion full cells by preformation of SEI layer on 3D binder-free anodes with and without Li metal.* ChemSusChem. 2015, 8(8):1368–1380.
6. Haitao Zhou, Xuehang Wang, De Chen. Li-Metal-Free Prelithiation of Si-Based Negative Electrodes for Full Li-Ion *Batteries*. ChemSusChem. 2015, 8(16): 2737-2744.

Financial support:

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

Mechanismistic research of light olefin formation in Fischer-Tropsch synthesis

PhD 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. Due to the crude oil demand and large reserves of natural gas and coal, FTS is an attractive industrial process. 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 recent years, density functional theory (DFT) calculations are widely used to investigate mechanisms by calculating the adsorption energy, activation energy and obtaining the potential energy diagram with high accuracy. While the DFT calculations will spend much time and be computationally expensive. The unity bond index-quadratic exponential potential (UBI-QEP) method, formerly known as the BOC-MP (Bond-order-conservation Morse-potential) method, is also a much used approach for calculation of adsorption heats and activation energies by using simple equations. However, low accuracy is a main problem for UBI-QEP method.

In order to enhance FTS light olefin production, this work aims for improved catalyst design based on a better understanding of the reaction mechanism on several different metal surfaces through combined DFT calculations, UBI-QEP method and microkinetic analysis. DFT calculations are performed by using the Vienna Ab-initio Simulation Package (VASP) code. The calculation is proceed firstly on the hcp (0001) surface of Cobalt, then applied in other metal surfaces, such as Fe, Ni, Pt, Pd, and so on. The reaction heats and activation energies for the elementary steps of light olefin formation are estimated by DFT calculations and UBI-QEP methods, respectively. In the previous work, UBI-QEP method has been modified which can satisfactorily fit the DFT estimated adsorption heats of different C1 and C2 products in FTS over various transition metal catalysts, including Co, Fe, Ni, Pt, Pd, Ru and Rh catalysts. It reduces radically the computational expenses, but keeps the accuracy compared to DFT calculation. C-, H- and O-metal binding energy are three sole descriptors for describing the adsorption and reactions on transition metal catalysts.

In the next work, a couple of modification of UBI-QEP equations will be applied to get a good relationship of activation energies for the elementary steps of light olefin formation between DFT results and modified UBI-QEP method. The modified UBI-QEP method will be used in the microkinetic analysis of

FTO reactions with O- and C-metal binding energy as descriptors. The initial values of rate constants will be determined by transition state theory for microkinetic model. A scaling relationship between activation energy (adsorption energy) and carbon number over different metal surfaces will be researched. The objective is to gain better understanding of the mechanism to achieve the goal of rational design of the catalysts.

This project is funded by NTNU.

Catalytic Conversion of Lignocellulosic Biomass to Chemicals and Fuels

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

Today, transportation fuels and chemicals are mainly produced from fossil carbon sources. Due to the declining reserves and environmental effects, a transition to renewable carbon sources, like biomass, is important. Conventional biomass sources, like starch and sugar, are easily exploitable, but have a too high fertilizer demand and are of too low abundance to be sustainable. Lignocellulosic biomass, such as trees, is the most abundant biomass and one of the most promising renewable carbon sources. It is however very complex and relatively resistant to chemical transformation, making it difficult to exploit. In recent years interesting, results have been published on using hot compressed water as a reaction medium for the conversion of lignocellulosic biomass. The hot compressed water has an excellent ability to facilitate the disintegration of lignocellulose, making it accessible for catalytic conversion into a variety of smaller oxygenates.

Our research is focused on developing the hot compressed water process. We want to develop catalytic systems to selectively convert lignocellulosic biomass into a variety of chemicals and fuels. We have investigated ZnO-coated CNT as a composite support for Ni and Cu catalyst. The composite support gives basic character and a large surface area. The large surface area provides the basis for a large metal-ZnO interphase and enhances the formation of alloys. The alloys proved to be highly active in the direct conversion of cellulose to vicinal diols, e.g. ethylene glycol and 1,2-propylene glycol, through the retro-aldol condensation. The same catalyst and reaction conditions were simultaneously used to convert the lignin fraction to its monomeric phenolic compounds, enabling this process to directly convert raw lignocellulosic biomass in one single step. The valorization of lignocellulosic biomass with hot compressed water can also be succeeded with an aldol condensation reaction were the smaller oxygenates produced can be directly converted into hydrocarbons by use of conventional catalyst providing a simple route to produce biofuels.

Publications and presentations in 2015:

1. C. van der Wijst, X. Duan, I. Skeie Liland, J. C. Walmsley, J. Zhu, A. Wang, T. Zhang, and D. Chen, *ZnO–Carbon-Nanotube Composite Supported Nickel Catalysts for Selective Conversion of Cellulose into Vicinal Diols*. ChemCatChem, 7 (2015) 2991–2999.
2. C. van der Wijst, X. Duan, I. Skeie Liland, J. C. Walmsley, J. Zhu, A. Wang, T. Zhang, and D. Chen, *CNT Supported Nickel-Zink Oxide Catalysts for Cellulose Conversion*. Oral Presentation. XII European Congress on Catalysis, Kazan, Russia, 2015.

Financial support: NTNU

Integrated H2BioOil process for efficient biofuel production

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

The increasing global concern about climate change and CO_2 emissions is calling for innovational research and development for new energy generation technologies from renewable (lignocellulose) resources. There are several path to produce fuel from lignocellulose biomass such as gasification, hydrolysis and pyrolysis. Pyrolysis of wood based biomass (lignocellulose), cheaply exploitable biomass source, produces low quality bio-oil due to its high acid value (TAN), oxygen content and energy density (16-19 MJ/kg). Therefore, to meet the transportation fuel standard, hydro-treating and catalytic upgrading is required.
Fast-hydropyrolysis (FHP) is a promising addition to the conventional pyrolysis. In this project, an in-situ generated H_2 gas and lignocellulose feedstock (pine) will be fed to the FHP reactor. The FHP reactor will be integrated with a catalytic reactor, having catalytic aldol condensation and hydrodeoxygenation (HDO) catalyst, to improve the fuel properties of the bio-oil. Thus, ketonization, aldol condensation (CAC) and hydrodeoxygenation (HDO) reactions will be optimized on cheaply and rationally designed Ni, Mo and Zn based bimetallic catalyst supported on Nitrogen doped CNT or hydrotalcite as well as TiO_2, Au/SiO_2 and Zeolite. Thus, embodies, applied catalyst design to activate ketonization, aldol condensation and hydrodeoxygenation reactions in the single reactor with a dual bed. In that, a systematic study in a continuous flow high

pressure reactor will be executed to understand the effects of process conditions on FHP as well as the downstream integrated catalytic aldol and Hydrodeoxygenation reactor.

Comprehensive catalyst characterization techniques such as TPD, XPS, STEM, FTIR, BET, and XRD etc. will be employed on the rationally designed catalyst while the product identification and quantification (activity and selectivity) will be done in an online GC-FID as well as GC-MS, and HPLC-MS.

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

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

Post.doc:	Dr. Diego Alexander Pena Zapata
Supervisor:	Prof. Magnus Rønning

Fischer-Tropsch Syntheses (FTS) for synthetic hydrocarbons production from coal and natural gas and biomass-derived syngas (X to liquids XTL 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 could result in 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. Therefore the optimization of catalyst performance is a very important issue. The 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 the decrease of catalyst deactivation with time on stream, which is one of the main challenges in industrial FTS applications.

The project aims to study the catalytic behavior of different FTS iron based catalysts activated under different gas atmosphere (CO, H_2, and syngas (H_2/CO=2)). Several catalyst systems are tested: supported iron, unsupported iron (bulk), promoted, un-promoted and iron carbide rich catalysts. Catalyst activity and stability are evaluated in a fixed bed reactor rig. A wide range of *ex-situ* and *in-situ* characterization techniques are used in order to reveal changes in active sites and iron phases under different gas pre-treatments (activation) and FT performance as well as understand the main role of deactivation mechanisms on catalysts lifetime. The catalyst before and after reaction are characterized 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* experiments such as X-ray Diffraction (XRD) and X-ray Absorption Spectroscopy (XAS) are performed during gas pre-treatment (activation) and FTS steps at the Swiss Norwegian beam Line (SNBL) in the European Synchrotron Radiation Facilities (ESRF) Grenoble, France. The results may have impact in a better catalyst activation protocol, active carbide phase identification and a deeper understanding of catalyst deactivation mechanisms.

Financial support: The work is financed by the European FP7 project FASTCARD (FAST industrialization by CAtalysts Research and Development), Grant agreement no: 604277. The research is part of work package 2 (WP2) on the development of next generation supported iron Fischer-Tropsch (FT) catalysts.

Presentations in 2015:

1. Diego Alexander Pena Zapata: *The effect of Cu Loading on carbide phase formation in Fe-based catalysts during Fischer-Tropsch Synthesis: in-situ XANES and XPD studies.* The 15th Norwegian Catalysis Symposium Bergen, 3-4 December 2015

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 R&D

Refinery operations / Octane processes

Staff: Research scientist Hilde Bjørkan, 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 RDI

Advanced Biofuel via Synthesis Gas

H_2S removal from biomass gasification gas

Staff: Research Scientist Svatopluk Chytil, Prof. Edd A. Blekkan (NTNU)

The project aim is to study the removal of H_2S from a model gasification gas using solid sorbents. Initially, manganese oxides on various supports were tested as H2S sorbent materials. Performance of the H_2S sorbents was assessed in an in-house built set-up and the emphasis was placed on the evaluation of sorbent capacity, stability over a number of sorption/ regeneration cycles and stability in a reducing atmosphere. Fresh, spent and regenerated sorbents were characterised using methods available in the KinCat centre. In the first part of the project a possible deactivation mechanism was proposed for the alumina supported manganese oxides used for the sorption removal of H_2S. In the second part, an attempt was made to clarify the influence of different supports (Al_2O_3, CeO_2, ZrO_2, TiO_2) on the sorption performance.

Publication in 2015:

1. Svatopluk Chytil, Milly Kure, Rune Lødeng and Edd A. Blekkan, *On the initial deactivation of MnxOy –Al2O3 sorbents for high temperature removal of H2S from producer gas*, Fuel Processing Technology, 133 (2015) 183
2. Svatopluk Chytil, Milly Kure, Rune Lødeng and Edd A. Blekkan, *H2S absorption on supported manganese oxides in dry reducing atmosphere*, submitted

Client: Research council of Norway

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

Utvikling av gassbasert industriklynge på Tjeldbergodden

Staff: Senior Scientist Bjørn Christian Enger, Research Manager Thor Bjørkvoll, Research Manager Heidi Bull-Berg, Senior Scientist Rune Lødeng, Research Manager Torbjørn Gjervan, Research Director Jack Ødegaard

The goal of this project was to develop a scenario for a natural gas based industry cluster at Tjeldbergodden based on its site assets.

Client: Tjeldbergodden Utvikling

FAST industrialisation by CAtalysts Research and Development (FASTCARD)

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

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

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

WP3 will develop such 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, $ZrO2$ 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

Philosphiae Doctor (PhD) theses in 2015

Andrey Volynkin: *The role of carbon supports in platinum catalyzed hydrogentation/dehydrogentation model reaction*. Doctorial thesis at NTNU, 2015:221

Ahn Hoang Dam: *Bimetallic catalyst system for steam reforming*. Doctorial thesis at NTNU, 2015:339

Disputas Andrey Volynkin 01.09.15. From left: Prof. Hallvard Svendsen, Prof. José Luís Figueiredo, Porto, Andrey Volynkin, Prof. Klaus J. Jens, University College South-East Norway, Prof. Edd A. Blekkan (supervisor), Prof. Magnus Rønning (supervisor)

Disputas Ahn Hoang Dahm 10.12.15. From left: Asc Prof. Hanna Knutilla, Prof. Zhixin Yu, UiS, Ahn Hoang Dahm, De Chen (supervisor), Prof. Lars J. Petterson, KTH, Prof. Edd A. Belekkan, Prof. Anders Holmen

Master (Diploma) Students in 2015

Sergiu Pareli; *Sorption of hydrogen chloride on solid sorbents*

Endre Fenes; *Kinetic Study of the Oxychloration Process*

Thomas Støme Hemminghytt; *Multifuctional proppants for enhanced oil production from shales*

Siri Foss Morken; *One-pot Conversion of Biomass to Chemicals on Ni-Cu/ZnO Based Catalysts*

Haakon Marius Vatten Rui; *Synthesis and Characterisation of Thungsten Carbide*

Hanne Marie Straume; *Cobalt/Manganese Oxide Nanoparticles for Enhanced Olefin Production in Fischer-Tropsch*

Astri Karin Torvik Jenssen; *Catalytic conversion of oxygenates to fules*

Isaac Yeboah; *Characterization and Thermal/Catalytic Upgrading of Kerogen in a Green River Oil Shale*

Anne Helene Barsnes; *Nitrogen-Doped Carbon Nanofibers as Pt-Free Catalysts in the Oxygen Reduction Reaction*

Øyvind Juvkvam Eraker; *Pressurized Reduction of Cu-ZnO Water-Gas-Shift-Catalysts in Presence of Water*

Hector Inglesias Gonzalez; *Photocatalytic H2-production through photo-reforming of hydrocarbons*

Lise Saue Jensen; *Synthesis Gas for the Fischer- Tropsch Sythesis*

Ata ul Rauf Salman; *Surface Modified γ-Alumina Supports for Cobalt Fischer-Tropsch Catalysts*

Stine Hagen Wigum; *Nickel and Iron Poisoning of Copper Based Methanol Synthesis Catalysts*

Nils-Olav Andersen Hole; *Effects of Potassium and Copper Promoters on Iron Fischer-Tropsch Catalysts*

Jihye Hwang; *Initial stages of metal dusting corrosion*

Linn Cecilie Sørvik; *Investigation of PdAu membranes and model systems for production of pure hydrogen.*

Kataryzina Swirk; *The surface properties of activated carbon as DeNOx catalysts modified by urea*

Group meetings with seminars

Location: K5-201

Day	Time	Presenter	Topic
February 13	14:00	**Hilde J. Venvik,** NTNU	Industrial Catalysis Science and Innovation forb a competitive and sustainable process industry
February 27	14:00	**Cristian Ledesma Rodriguez,** NTNU	Identification of the Reaction Network of Fischer-Tropsch Synthesis by Multicomponent Isotopic Transient Methods
March 13	10:15 14:15	**Dr. Maximilian Warner,** Yara	The kinetics of industrial ammonia combustion The Ostwald process, and how to teach an old dog new tricks
April 10	14:00	**Martina Baidoo,** NTNU	Kinetic study of the oxychlorination process
April 24	14:00	**Cornelis van der Wijst,** NTNU	Conversion of biomass to chemicals and fuels
May 8	14:00	**Xuezhi Duan,** NTNU	Catalytic conversion of kerogen
May 22	14:00	**Fengliu Lou,** NTNU	Synthesis and application of N-doped graphene
June 5	14:00	**Ida Hjort,** NTNU	Progresses in researches for solar fuels
June 19	14:00	**Esther Acha Peña,** University of the Basque Country	From SUPREN to KINCAT

Day	Time	Presenter	Topic
August 14	14:00	**Jong-Min Lee,** Nanyang Technological University (NTU), Singapore	Some applications of Electrochemistry and Green Chemistry
August 28	14:00	**Ikko Mikami,** Tokai University, Japan	Catalysts and photocatalysts for water treatment
September 15	14:15	**Dr. Fei Chen,** HTAS	Making optimal performance possible -Introducing Haldor Topsøe AS
September 25	14:00	**Di Wang,**	Modified carbon nanotubes by $KMnO_4$ supported iron Fischer-Tropsch catalyst for direct conversion of syngas to lower olefins
October 23	14:00	**Edvard Bergene,** Statoil	Troubleshooting CO_2 driers at Snøhvit, story of a solved case
November	14:00	**Ivan Ivanov Bogoev,**	Gold based catalysts on ceria and ceria-

13		Institute of Catalysis, Bulgarian Academy of Sciences	metal oxides for WGS reaction (WGS gold catalysts)
November 20	14:00	**Anh Hoang Dam,** NTNU	Bimetallic Catalyst System for Steam Reforming
December 11	13:00	**Lars J Pettersson,** KTH, Sweden	The Black Gold - From Whales to Texas

Courses given by Group Members

TKP4110 Chemical Reaction Engineering

Coordinator: Professor Jens-Petter Andreassen

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

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

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

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

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

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

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

Exam: Written + exercises

TKP4150 Petrochemistry and oil refining

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

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

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

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

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

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

Teaching:

The course is given as a combination of lectures, exercises, self-study and project work including student presentations.
Course material:
J. Moulijn, M. Makkee and A. van Diepen: Chemical Process Technology Wiley & Sons, 2001, articles and handouts.

Exam: Written

TKP4155 Reaction Kinetics and Catalysis

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

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

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

Prerequisites:
Course TKP4110 Chemical Reaction Engineering or similar knowledge.

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

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

Course material:

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

Exam: Written

TKP4190 - Fabrication and Applications of Nanomaterials

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

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

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

Prerequisites:
Basis chemistry and mathematics and course TMT4320 Nanomaterials.

Contents:
The thermodynamic driving force and the kinetics of nucleation and growth of nanoparticles is derived, focusing on precipitation from solutions. Different mechanism for nucleation and crystal growth along with calculations of nucleation and growth rates define the basis for design of different particle populations and applications relevant to research and industry.
The unique optical properties of nanoparticles made of noble metals such as gold and silver (localized surface plasmon resonance, LSPR), and how these can be implemented in detection and diagnostic applications via molecular spectroscopy. Use of nanomaterials such as gold nanoparticles, dendrimers, carbon nanotubes and plant viruses for medical applications such as chemotherapy and gene therapy.
Methods for the fabrication of catalysts and catalyst supports based on precipitation, along with other methods with particular relevance for the catalyst nanostructure and functionality, such as sol-gel and colloid based fabrication. Relevant examples where the significance of particle and pore size has been shown are included (Au, Co, Ni- catalysts and carbon nano fibres (CNF)). A

short introduction to catalytic model systems and surface science and their experimental and theoretical application within nanocatalysis.

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

TKP4190 – Introduction to nanotechnology

Responsible: Professor Helge Weman, Department of Electronics and Telecommunications

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

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

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

Prerequisites: None

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

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

Catalysis and petrochemistry MSc specialization

Coordinator: Professor Edd Anders Blekkan

Course description:

The specialization involves the following modules:

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

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

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

Responsible: Professor Hilde J. Venvik

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

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

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

Teaching methods: Seminars

Course material: Handouts

TKP4515-1 Heterogeneous catalysis, advanced course

Responsible: Professor Edd Anders Blekkan

Credits: 3.75 SP

Prerequisites:
TKP4155 Reaction kinetics and catalysis or similar knowledge.

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

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

Course material:
Articles and excerpts from textbooks.

Language:
English

KP4515-2 Environmental and energy catalysis

Responsible: Professor Hilde J. Venvik

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

Module description:
Catalysis occupies an important position within areas such as environmental technology and energy production. Within environmental technology catalysis has become crucial not only for removing of unwanted components such as NOX, sulfur etc., but also for the development of selective processes. The course will give the fundamentals for catalytic processes for purification of

exhaust gases (NOX, CO, unburned hydrocarbons etc). Within energy production the focus is on biofuel production, catalytic combustion, production of H2 and catalysis/reactor technology related to fuel cells. Catalysis for clean production will also be an important part of the course.

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

Course material:
Articles and excerpts from textbooks.

Language:
English

Ph.D. courses

KP8132 Applied heterogeneous catalysis

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

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

Course description:
The course is given every second year, next time in the fall term 2015.
The course gives an introduction to modern theories for the most important groups of heterogeneous catalysts: Metals, metal oxides and zeolites. Examples of industrial applications are included. An overview of the principles for design and preparation of heterogeneous catalysis will be given. The course includes a kinetic description of the different processes involved in a catalytic cycle: Adsorption, surface reaction and desorption in addition to mass and heat transfer. An introduction to different experimental methods for studying catalytic reactions will also be given.

Teaching methods:
Seminars.

Course material:
Selected articles and handouts.

KP8133 Characterization of heterogeneous catalysts

Responsible: Professor Magnus Rønning

Credits: 7.5 SP

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

Course material:
Selected scientific papers.

KP8136 - Modelling of Catalytic Reactions

Responsible: Professor De Chen

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

Course description:
The course is given every second year, next time in spring 2015
The course gives an overview on the methods for building microkinetic model, collecting or theoretically estimating rate constant, and microkinetic simulation. Focus will also on the microkinetic analysis of reaction systems at the atomic level. A project work of microkinetic modeling of a selected reaction system will be included in the course.

Learning methods and activities:
Seminars + project

Course materials:

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

KP8137 - Design and Preparation of Catalytic Materials

Responsible: Professor Hilde Johnsen Venvik
Lecturer: Professor Edd Blekkan

Credits: 7.5 SP

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

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

Learning methods and activities:
Seminars

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

Course materials:
Selected handouts and scientific papers

Publications in 2015

1. Yanying Qi, Jia Yang, De Chen, Anders Holmen: *Recent Progresses in Understanding of Co-Based Fischer-Tropsch Catalysis by Means of Transient Kinetic Studies and Theoretical Analysis*. Catal. Lett. 145 (2015) 145 – 161.
2. Erling Rytter, Anders Holmen: *Deactivation and Regeneration of Commercial Type Fischer-Tropsch Co-Catalysts-A Mini-Review.* Catalysts 5 (2015) 478-499
3. H. Romar, A.H. Lillebø, P. Tynjälä, T. Hu, A. Holmen, E.A. Blekkan, U. Lassi: *Characterization and Catalytic Fischer-Tropsch Activity of Co-Ru and Co-Re Catalysts Supported on* γ*-*Al_2O_3*,* TiO_2 *and SiC.* Top. Catal. 58 (2015) 887-895
4. J. Zhu, M.-L. Yang, Y. Yu, Y.-A. Zhu, Z.-J. Sui, X.-J. Sui, X.-G. Zhou, A. Holmen, D, Chen: *Size-Dependent Reaction Mechanism and Kinetics for Propane Dehydrogenation over Pt Catalysts.* ACS Catalysis 9 (2015) 6310-6319.
5. K.S Sultana, T.D. Tran, J.C. Walmsley, M. Rønning, D. Chen, *CaO Nanoparticles Coated by ZrO2 Layers for Enhanced CO2 Capture Stability*, Ind. Eng. Chem. Res. 54(2015) 8929-8939
6. P.P.C. Udani, M. Rønning, *Comparative study on the photocatalytic hydrogen production from methanol over Cu, Pd, Co and Au loaded TiO2*, Oil Gas Sci. Technol. (2015), 70 (5), 831-839
7. D. Chen, M. Rønning, *Preface*, Catal. Today, 249 (2015)
8. Volynkin, M. Rønning, E.A. Blekkan, *The role of carbon support for propane dehydrogenation over platinum catalysts*, Topics in Catalysis 58(14), (2015) 896-904
9. G. Voss, J. Bø Fløystad, A. Voronov, M. Rønning, *The State of Nickel as Promotor in Cobalt Fischer–Tropsch Synthesis Catalysts,* Topics in Catalysis, 58(14), (2015), 896-904
10. N.E. Tsakoumis, A.P.E. York, D. Chen, M. Rønning, *Combining reaction kinetics and catalyst characterization in one set-up: The state of the art*, Catal. Sci. Technol. 5 (2015) 4859-4883
11. T.O. Eschemann, W.S. Lamme, R.L. Manchester, T.E. Parmentier, A. Gognigni, M. Rønning, K.P. de Jong, *Effect of support surface treatment*

on the synthesis, structure and performance of Co/CNT Fischer-Tropsch catalysts, J. Catal. 328 (2015) 130–138

12. K. Swirk, M. Rønning, B. Samojeden, *Influence of the amount of urea modification of activated carbon on DeNOx catalyst efficiency,* Environmental Protection and Energy III (2015), 151-162. ISBN: 978-83-942601-2-5
13. Svatopluk Chytil, Milly Kure, Rune Lødeng, Edd A. Blekkan, *On the initial deactivation of MnxOy-Al2O3 sorbents for high temperature removal of H2S from producer gas,* Fuel Processing Technology 133 (2015) 183 – 194
14. Chen, De; Rønning, Magnus. *Preface*. *Catalysis Today* 2015; Volum 249.
15. Chen, Wenyao; Duan, Xuezhi; Qian, Gang; Chen, De; Zhou, Xinggui. *Carbon Nanotubes as Support in the Platinum-Catalyzed Hydrolytic Dehydrogenation of Ammonia Borane*. *ChemSusChem* 2015; Volum 8. (17) s.2927-2931
16. Duan, Xuezhi; Ji, Jian; Qian, Gang; Zhou, Xinggui; Chen, De.*Recent advances in synthesis of reshaped Fe and Ni particles at the tips of carbon nanofibers and their catalytic applications*. *Catalysis Today* 2015; Volum 249. s.2-11
17. Fan, Chen; Zhu, Yi-An; Yang, Ming-Lei; Sui, Zhi-Jun; Zhou, Xing-Gui; Chen, De. *Density Functional Theory-Assisted Microkinetic Analysis of Methane Dry Reforming on Ni Catalyst*. *Industrial & Engineering Chemistry Research* 2015; Volum 54. (22) s.5901-5913
18. Feng, Xiang; Duan, XueZhi; Cheng, Hong-ye; Qian, Gang; Chen, De; Yuan, Wei-Kang; Zhou, Xing-Gui. *Au/TS-1 catalyst prepared by deposition–precipitation method for propene epoxidation with H2/O2: Insights into the effects of slurry aging time and Si/Ti molar ratio*. *Journal of Catalysis* 2015; Volum 325. s.128-135
19. Feng, Xiang; Duan, Xuezhi; Yang, Jia; Qian, Gang; Zhou, Xinggui; Chen, De; Yuan, Weikang. *Au/uncalcined TS-1 catalysts for direct propene epoxidation with H2 and O2: Effects of Si/Ti molar ratio and Au loading*. Chemical Engineering Journal 2015; Volum 278. s.234-239
20. Gil Matellanes, Maria Victoria; Fermosi, Javier; Rubiera, Fernando; Chen, De. *H2 production by sorption enhanced steam reforming of biomass-derived bio-oil in a fluidized bed reactor: An assessment of the effect of operation variables using response surface methodology*. Catalysis *Today* 2015; Volum 242. s.19-34
21. Kazi, Saima Sultana; Tran, Trung Dung; Walmsley, John; Rønning, Magnus; Chen, De. *CaO Nanoparticles Coated by ZrO2 Layers for*

Enhanced CO2 Capture Stability. Industrial & Engineering Chemistry Research 2015; Volum 54. (36) s.8929-8939

22. Lou, Fengliu; Buan, Marthe Emelie Melandsø; Muthuswamy, Navaneethan; Walmsley, John; Rønning, Magnus; Chen, De.*One-step electrochemical synthesis of tunable nitrogen-doped graphene.* Journal of Materials Chemistry *A* 2015; Volum 4. (4) s.1233-1243
23. Lou, Fengliu; Chen, De.*Aligned carbon nanostructures based 3D electrodes for energy storage*. Journal of Energy Chemistry 2015; Volum 24. (5) s.559-586
24. Mahmoodinia, Mehdi; Åstrand, Per-Olof; Chen, De. *Chemical Bonding and Electronic Properties of the Co Adatom and Dimer Interacting with Polyaromatic Hydrocarbons*. Journal of Physical Chemistry C 2015; Volum 119. (43) s.24425-24438
25. Pham, Tranh Hai; Qi, Yanying; Yang, Jia; Duan, Xuezhi; Qian, Gang; Zhou, Xinggui; Chen, De; Yuan, Weikang. *Insights into Hägg Iron-Carbide-Catalyzed Fischer–Tropsch Synthesis: Suppression of CH4 Formation and Enhancement of C-C Coupling on XFe5C2 (510*). ACS Catalysis 2015; Volum 5. (4) s.2203-2208
26. Qi, Yanying; Yang, Jia; Chen, De; Holmen, Anders. *Recent Progresses in Understanding of Co-Based Fischer–Tropsch Catalysis by Means of Transient Kinetic Studies and Theoretical Analysis.* Catalysis Letters 2015; Volum 145. (1) s.145-161
27. Shan, Yuling; Sui, Zhijun; Zhu, Yian; Chen, De; Zhou, Xing-gui. *Effect of steam addition on the structure and activity of Pt–Sn catalysts in propane dehydrogenation*. Chemical Engineering Journal 2015 ;Volum 278. s.240-248
28. Shan, Yuling; Zhu, Yi-An; Sui, Zhi-Jun; Chen, De; Zhou, Xing-Gui. *Insights into the effects of steam on propane dehydrogenation over a Pt/Al2O3 catalyst*. Catalysis science & technology 2015; Volum 5.(8) s.3991-4000
29. Sun, Xiaoyan; Ding, Yuxiao; Zhang, Bingsen; Huang, Rui; Chen, De; Su, Dang Sheng. *Insight into the Enhanced Selectivity of Phosphate-Modified Annealed Nanodiamond for Oxidative Dehydrogenation Reactions*. ACS Catalysis 2015; Volum 5. (4) s.2436-2444
30. Tsakoumis, Nikolaos; York, Andrew P.E.; Chen, De; Rønning, Magnus. *Catalyst characterisation techniques and reaction cells operating at realistic conditions; towards acquisition of kinetically relevant information.* Catalysis science & technology 2015; Volum 5.(11) s.4859-4883
31. Van der Wijst, Cornelis; Duan, Xuezhi; Liland, Ingvild Skeie; Walmsley, John; Zhu, Jun; Wang, Aiqin; Zhang, Tao; Chen, De. *ZnO-Carbon-Nanotube Composite Supported Nickel Catalysts for Selective*

Conversion of Cellulose into Vicinal Diols. ChemCatChem 2015;Volum 7.(18) s.2991-2999

32. Wang, Di; Zhou, Xiangping; Ji, Jian; Duan, XueZhi; Qian, Gang; Zhou, Xing-Gui; Chen, De; Yuan, Wei-Kang. *Modified carbon nanotubes by KMnO4 supported iron Fischer-Tropsch catalyst for the direct conversion of syngas to lower olefins*. Journal of Materials Chemistry *A* 2015; Volum 3.(8) s.4560-4567
33. Yang, Jia; Frøseth, Vidar; Chen, De; Holmen, Anders. *Particle size effect for cobalt Fischer–Tropsch catalysts based on in situ CO chemisorption*. Surface Science 2015
34. Yang, Ming-Lei; Fan, Chen; Zhu, Yi-An; Sui, Zhi-Jun; Zhou, Xing-Gui; Chen, De. *Selective Oxidation of Hydrogen in the Presence of Propylene over Pt-Based Core-Shell Nanocatalysts*. Journal of Physical Chemistry *C* 2015;Volum 119.(37) s.21386-21394
35. Zhou, Haitao; Wang, Xuehang; Chen, De. *Li-metal-free prelithiation of Si-based negative electrodes for full Li-ion batteries*. ChemSusChem 2015; Volum 8.(16) s.2737-2744
36. Zhou, Haitao; Wang, Xuehang; Sheridan, Edel; Chen, De. *Boosting properties of 3D binder-free manganese oxide anodes by preformation of a solid electrolyte interphase*. ChemSusChem 2015; Volum8.(8) s.1368-1380
37. Zhou, Xiangping; Ji, Jian; Wang, Di; Duan, XueZhi; Qian, Gang; Chen, De; Zhou, Xing-Gui. *Hierarchical structured -Al2O3 supported S-promoted Fe catalysts for direct conversion of syngas to lower olefins*. Chemical Communications2015;Volum 51.(42) s.8853-8856
38. Zhu, Jun; Yang, Ming-Lei; Yu, Yingda; Zhu, Yi-An; Sui, Zhi-Jun; Zhou, Xing-Gui; Holmen, Anders; Chen, De.*Size-Dependent Reaction Mechanism and Kinetics for Propane Dehydrogenation over Pt Catalysts*. ACS Catalysis 2015;Volum 5.(11) s.6310-6319

Presentations in 2015

1. A Holmen. B.C. Enger, A. Helland Lillebø, E.A. Blekkan: *Nickel aluminate/α-alumina as catalysts for partial oxidation and as support for cobalt Fischer-Tropsch catalysts*. Lecture. 249th ACS National Meeting & Exposition, March 22-26, 2015 Denver, USA.
2. Y. Qi, J. Yang, Y. Zhu, D. Chen A. Holmen: *Mechanistic Studies of Cobalt-Catalyzed Fischer-Tropsch Isotopic Effect and Kinetic Analysis.* Poster. NAM 24, June 14-19, 2015 Pittsburgh, USA.
3. C. Ledesma, J. Yang. E.A. Blekkan, A. Holmen, D. Chen*: *Identifying the Kinetic Parameters of Fischer-Tropsch Synthesis over Cobalt-Rhenium/CNT Catalyst by Isotopic Transient Methods*. Lecture. NAM 24, June 14-19, 2015 Pittsburgh, USA.
4. C. Ledesma, J. Yang. E.A. Blekkan, A. Holmen, D. Chen*: *Study of Reaction Network of Fischer-Tropsch Synthesis by Multicomponent Steady_State Isotopic Transient Kinetic Analysis*. Poster. EuropaCat XII, August 30 – September 4, 2015, Kazan, Russia.
5. L. Gavrilovic, E.A. Blekkan, A. Holmem, H.J. Venvik, J. Brandin: *Fischer-Tropsch Synthesis – Investigation of Co catalyst by exposure to aerosol particles of potassium salts*. Thew 15th Norwegian Catalysis Symposium, December 3-4 2015, Bergen.
6. Mahmoodinia, Mehdi; Ebadi, Mahsa; Åstrand, Per-Olof; Chen, De. *Atomic and electronic structure of transition metal-graphene nanoflake interactions*. The 15th International Congress of Quantum Chemistry; 2015-06-08 - 2015-06-13
7. Mahmoodinia, Mehdi; Åstrand, Per-Olof; Chen, De. *Density Functional Study of CO Adsorption on Edge-Functionalized Graphene-Supported Pt Clusters*. Annual Meeting in Quantum and Computational Chemistry; 2015-06-29 - 2015-06-30
8. Mahmoodinia, Mehdi; Åstrand, Per-Olof; Chen, De. *Reactivity of metal atoms and clusters on carbon surfaces: Insights from Reax simulations and DFT calculations*. Pacifichem; 2015-12-15 - 2015-12-20
9. M. Rønning, M.E.M. Buan, N. Muthuswamy, D. Chen, *Nitrogen-doped carbon nanomaterials as alternative catalysts for the Oxygen Reduction Reaction*, Keynote lecture; Norwegian Catalysis Symposium, December 3-4. 2015, Bergen, Norway

10. M. Rønning, SNBL: *Celebrating 20 Years of Catalyst Characterisation Development*, SNBL 20 Years Anniversary Workshop, May 28 – 29. 2015, Grenoble, France
11. M. Rønning, *Replacing platinum group metals with N-doped carbon nanomaterials in the oxygen reduction reaction*, Aalto University, April 10. 2015, Helsinki, Finland
12. M. Rønning, *FREECATS: Doped carbon nanostructures as metal-free catalysts*, CRM InnoNet 3rd Innovation Network Workshop, February 11. 2015, Brussels, Belgium
13. 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)
14. Qi, Yanying; Yang, Jia; Chen, De; Holmen, Anders. *Mechanistic studies of cobalt-catalyzed Fischer-Tropsch synthesis by a combined approach of DFT calculations, kinetic isotope effect and kinetic analysis*. 24th North American Catalysis Society Meeting; 2015-06-14 - 2015-06-19

KinCat
Catalysis Group – SINTEF – NTNU

KINCAT Seminar Friday 11 December 2015

The Black Gold - From Whales to Texas

Speaker **Professor Lars J. Pettersson**
Department of Chemical Engineering and Technology
KTH Royal Institute of Technology
Stockholm, Sweden
Date Friday, 11 December 2015 at 13:00
Venue Auditorium R3, Realfagsbygget

Abstract

This seminar in chemical engineering, with the focus on the history of technology, will take you back to the birth of the oil industry in the 19th century in Pennsylvania and also in Azerbaijan. The focus will be on the first dynamic period 1850-1920. The endpoint of the seminar is set to when the Texas oil fields became the World leader in supplying oil to a mass market. I will try to answer the question why whaling became so important for a new feedstock to evolve. In the course of this seminar you will meet several colourful people, such as “Colonel” Drake, and the so called Robber Barons John D. Rockefeller, Andrew Carnegie and Henry Clay Frick. The last person was called the most hated man in America. Why was that? We will also look into what Alfred Nobel´s two older brothers Robert and Ludvig accomplished in Baku. Who were these people and how did they influence the transformation of the society? Which societal needs triggered the development? Why did crude oil become the dominating hydrocarbon feedstock for automotive applications? Which were the innovations that paved the way for the establishment of an oil industry? The importance of safe explosives in the development of this industry will also be discussed. Last but not least, who was Miss Margarine?

Trial Lectures for the PhD degree

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

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

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

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

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

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

Ola Olsvik: *Catalytic membrane reactors*. 1993

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Magnus Rønning: *Photocatalysis*. 2/3 2000

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

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

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

Lucie Bednarova: *Computational Catalysis*. 2002

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

Leiv Låte: *Catalysis in supercritical fluids*. 2002

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

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

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

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

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

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

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

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

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

Erlend Bjørgum: *Photocatalysis* 20/1 2006

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

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

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

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

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

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

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

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

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

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

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

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

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

Sara Boullosa Eiras: *Catalysts and materials development in solid oxide fuel cells*. 22/10 2010
Hamidreza Bakhtiary; *Production of* C_2-C_4 *alcohols from synthesis gas*. 3/11 2010.

Xuyen Kim Phan: *Direct catalytic conversion of carbohydrates to hydrocarbons*. 2001

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Alumni
PhD students Catalysis group:

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Petr Steiner
Kinetic and deactivation studies of hydrodesulfurization catalysts
Defense of thesis: December 2002
Current position: Director, Downstream at Stratas Advisors, Hart Energy Consulting, Belgium.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Ingvar Kvande
Carbon nanofiber supported platinum catalysts.
Defense of thesis: December 2007
Current position: Researcher, Bioforsk Økologisk, Tingvoll

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

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

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

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

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

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

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
Current position: Trondheim Forskning og Utvikling (TFoU)

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: Researcher, SINTEF

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

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Calcium Based CO_2 Acceptors for Sorption Enhanced Steam Methane Reforming
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Platinum based Catalysts for Methanol Fuel Cells: Metal Clusters and Carbon Supports.
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Current positions: Post.doc. NTNU

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

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

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

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

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Aligned carbon nanotubes@manganese oxide coaxial arrays for lithium ion batteries.
Defense of thesis: September 2013
Current position: Post.doc. NTNU

Daham Sanjaya Gunawardana Panditha Vidana
Carbon formation phenomena and the initial stage of metal dusting corrosion - an experimental investigation
Defense of thesis: January 2014
Current position: Post.doc. NTNU

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

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

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

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

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

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