

# Annual Report

2018



Catalysis Group – SINTEF – NTNU

**KinCat**  
**Strong Point Centre Kinetics and Catalysis**

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

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**Annual Report 2018**  
**KINCAT**  
**Strong Point Centre Kinetics and Catalysis**

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**KinCat Members**  
**Catalysis Group, Department of Chemical Engineering**

Academic staff:

Professor Edd A. Blekkan  
Professor De Chen  
Professor Magnus Rønning  
Professor Hilde J. Venvik  
Assoc. Professor Jia Yang  
Professor Em. Anders Holmen  
Professor Em. Erling Rytter  
Adjunct Professor Kjell Moljord  
Adjunct Assoc. Prof. Ingeborg-Helene Svenum

SFI-coordinators:

Coordinator Estelle Marie M. Vanhaecke (50%)  
Coordinator Nikolaos Tsakoumis (20% from 01.08 2018-31.05.19)  
Coordinator Anne Hoff (30% from 06.08 2018-06.05.19)

Laboratory personnel:

Engineer Karin Wiggen Dragsten (to 05.09.19)  
Senior Engineer Estelle Vanhaecke (50%)  
Senior Engineer Anne Hoff (70% from 06.08 2018-06.05.19)

Doctoral students 2018/2019:

Martina Francisca Baidoo	Samuel Regli
Ole H. Bjørkedal	Haakon Rui
Endre Fenes	Ata ul Rauf Salman
Ljubisa Gavrilovic	Yalan Wang
Xiaoyang Guo	Cornelis Gerardus van der Wijst
Stine Lervold	Isaac Yeboah
Yahao Li	Daniel Skodvin
Shirley Elisabeth Liland	Hongfei Ma
Juntian Niu	Jianyu Ma
Eirik Østbye Pedersen	Muhammad Zubair
Joakim Tafjord	Moses Mawanga
Martina Cazzolaro	Mario Ernesto Casalegno
Jibin Antony	

Postdoctoral fellows/Researchers 2018/2019

Qingjun Chen	Xiang Feng
Mari Helene Farstad	Nikolaos Tsakoumis
Li He	Shirley Elisabeth Liland
Jørgen Svendby	Zhenping Cai
Ljubisa Gavrilovic	Ainara Moral Larrasoana
Yanying Qi	Xiaoyang Guo
Marie Døvre Strømsheim	

Visitors 2018/2019

Bingxu Chen	Nianju Hou
Katarzyna Swirk	Weixin Qian
Mehdi Mahmoodina	Xiaoli Yang

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

Harry T. Brun, retired 30.06.2018	Mikael Hammer
Jan Morten Roel, retired 31.07.2018	Erland Strendo
Gunn Torill Wikdahl	Ketil Torset Helland

**SINTEF Industry, Department of Kinetics and Catalysis**

Administration:

Research Manager Torbjørn Gjervan  
Senior-/Project Secretary Kirsti Blomsøy

Research scientists:

Research Scientist Håkon Bergem  
Research Scientist Hilde Bjørkan  
Senior Scientist Bjørn Christian Enger  
Senior Scientist Rune Lødeng  
Research Scientist Rune Myrstad  
Research Scientist Kumar R. Rout

Laboratory personnel

Senior Engineer Camilla Otterlei



5<sup>th</sup> row: Joakim Tafjord, Ljubisa Gavrilovic,

4<sup>th</sup> row: Ole Bjørkedal, Mario Ernesto Casalegno, Mehdi Mahmoodinia, Daniel Skodvin, Ata ul Rauf Salman, Yuanwei Zhang, Jibin Antony, Jiayu Ma, Rune Myrstad, Magnus Rønning, Bjørn Christian Enger, Xiaoyang Guo, Anders Holmen,

3<sup>rd</sup> row: Håkon Bergem, Hongfei Ma, Rune Lødteng, Camilla Otterlei, Moses Mawanga, Weixin Qian, Hilde Bjørkan, Edd Blekkan, Suresh Kannan Balasingam, Zhenping Cai

2<sup>nd</sup> row: Jia Yang, Hilde Venvik, Marie Døvre Strømsheim, Yanying Qi, Shirley Liland, Anne Hoff,

1<sup>st</sup> row: Martina Cazzolaro, Asma Hayoune, Yalan Wang, Estelle Vanhaecke, Ainara Moral Larrasoana, Nikolaos Tsakoumis

Not present: De Chen, Kjell Moljord, Torbjørn Gjervan, Kumar Rout, Muhammad Zubair, Stine Lervold, Jørgen Svendby, Endre Fenes, Erling Rytter, Xiaoli Yang, Nianju Hou, Samuel Regli, Xiang Feng,

## Research Areas

### ❖ Conversion of Natural Gas

- Synthesis gas and hydrogen production
- Fischer-Tropsch synthesis
- Dehydrogenation of ethane and propane
- Solid acceptors for CO<sub>2</sub>-capture
- Production of methanol and dimethyl ether (DME)
- Direct methane conversion

### ❖ Industrial catalysis

- Oxychlorination
- Catalytic oxidation of NO to NO<sub>2</sub>
- Catalytic oxidation of methanol to formaldehyde

### ❖ Upgrading of Oil Fractions

- Hydrotreating
- Catalytic reforming/isomerization

### ❖ Biofuels

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

### ❖ High Temperature Chemistry

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

### ❖ Environmental Catalysis

- Sulfur reduction by hydrotreating
- Oxidation of CO and hydrocarbons
- CO<sub>2</sub> conversion
- NO<sub>x</sub> abatement

### ❖ Fundamental Studies of Heterogeneous Catalysis

- Surface science and *in situ* methods
- Preparation of catalytic materials (supported metals and metal oxides, zeolites, supports, nanoparticles)

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

❖ **Microstructured Reactors and Membrane Reactors**

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

❖ **Gas cleaning**

- Sorbent and processes for H<sub>2</sub>S removal.
- Sorbents and processes for CO<sub>2</sub> capture.

❖ **Photocatalysis**

- Water splitting
- Photoreforming
- Nitrogen fixation



## Main Laboratory Equipment

### ❖ Reaction Laboratories

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

### ❖ Catalyst Preparation Laboratory

- Spray drier
- Ball mills
- Furnaces
- Granulation equipment
- Calcination set-up
- High Temperature ovens
- Rotary evaporator

### ❖ Catalysts and Products Characterization

- Surface area (BET), porosity and pore size distribution
- Chemisorption and adsorption calorimetry
- Temperature programmed methods such as TPR, TPO and TPD, Acidity determination by TPD (Altamira BenchCat Hybrid)
- TGA-MS and DSC
- Raman (*ex-situ* and *in-situ*)
- FT-IR (*in-situ*)
- Pyrolysis GC-MS
- GC-MS, micro-GC, MS and HPLC
- XRF – X-ray fluorescence
- Scanning tunneling microscopy (STM)
- The following methods are available at NTNU:  
EM (electron microscopy), XPS (X-ray photoelectron spectroscopy), AES (auger electron spectroscopy), NMR, AFM (atomic force microscopy) and XRD (X-ray diffraction).
- Synchrotron radiation EXAFS and XRD are frequently used through ESRF and other facilities.
- Synchrotron radiation HR-PES and APPES are frequently used through MAXIV, ASTRID2 and other facilities.

## Highlights from the Activities in 2018

- ❖ Three candidates completed their PhD degrees in 2018: Yahao Li, Ljubisa Gavrilović and Erik Østbye Pedersen. The titles of the dissertations, the title of the trial lectures and pictures of the candidates/committees/ supervisors are enclosed
- ❖ 20 NTNU and 3 exchange M.Sc students completed their thesis in 2018. Their name and titles are enclosed.
- ❖ Professor De Chen had a one-year Sabbatical leave for 2017/2018 in China. Adjunct Assoc. Professor Ingeborg-Helene Svenum is on a one year Sabbatical Leave for 2018/2019 in Madison, USA.
- ❖ iCSI – industrial Catalysis Science and Innovation – is a Centre for Research-based Innovation awarded by the Research Council of Norway (SFI) with the industrial partners Yara, KA Rasmussen, Dynea, Inovyn, and Haldor Topsøe, and the academic partners are NTNU, UiO and SINTEF. NTNU is the Centre host with Professor Hilde Venvik as the Centre manager. A description of iCSI is enclosed.
- ❖ The Annual Meeting of ICSI was organized on 19<sup>th</sup> and 20<sup>th</sup> November 2018 at Selbusjøen Hotel og Gjestegård. The program is enclosed.
- ❖ The group is a research partner in BIO4FUELS, a Centre for Environment -friendly Energy Research (FME), hosted by The Norwegian University of Life Sciences (NMBU). The Center has a total budget of around 270 MNOK over 8 years and covers all important value-chains for conversion of lignocellulosic biomass to biofuels. User partners are key national and international industries, as well as forestry owners and regional authorities. Our activities are related to catalytic processes for the production of biofuels and chemicals from biomass.
- ❖ The group was the conference host of the 11<sup>th</sup> Natural Gas Conversion Symposium (NGCS11) in Tromsø June 5-9 2016. The Special Issue of Catalysis Today with selected papers from NGCS11 was finalized in 2018 with Hilde Venvik, Anders Holmen, De Chen, Erling Rytter and Duncan Akporiaye as Guest Editors.
- ❖ 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.
- ❖ 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.
- ❖ The group awarded financial support for equipment for biomass conversion under the Norbiolab-project.

## Awards

KinCat researchers recently received recognition at the International Conference on Chemical Reaction Engineering (ISCRE 25) in Firenze, Italy, with more than 500 participants from worldwide. KinCat principal investigator Professor De Chen (NTNU) gave a keynote lecture entitled “Kinetic Analysis and Design of Catalytic Redox Cycles” that was very well received and attracted attention.



Moreover, SINTEF Research scientist Dr. Kumar R. Rout received special recognition for his contribution submitted to the Gianni Astarita Young Investigator Award Committee. This award recognizes “a young researcher for his/her outstanding research in Chemical Reaction Engineering”.

Two PhD candidates received Poster awards:

Stine Lervold received the Best Poster Award for her work on "Morphology study of electrolytic silver catalyst for partial oxidation of methanol to formaldehyde (MTF)" at the 18th Nordic Symposium on Catalysis in Copenhagen, from 26-28 August.



Samuel Regli received a Poster Award in recognition of outstanding poster presentation at XAFS2018, Kraków, Poland.

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

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

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



UiO : Universitetet i Oslo

 **SINTEF**

inovyn

K.A.Rasmussen  
Norway**HALDOR TOPSØE** 

2018 was a year of recognition for iCSI, during which our young scientists and seniors showed their innovation potential by disseminating high quality research from the Centre. iCSI researchers gave 22 presentations at national and international conferences. Furthermore, iCSI partners acquired 6 national and European grants.

Some iCSI team members had particularly high international visibility during 2018. Three of the iCSI young scientists received best poster awards in different events, and 2 seniors were recognized for their contribution to catalysis and chemical reaction engineering. An absolute highlight was the announcement of the Awardee for Excellence in Natural Gas Conversion 2019, who is no other than iCSI professor Unni Olsbye; becoming the first woman included to the hall of fame of natural gas conversion.

iCSI researchers publish their findings and perspectives in high impact journals such as Journal of the American Chemical Society and Chemical Society Reviews. While the IIA 4 and IIA 5 are leading the way, it is nice to see that high-quality research results and publications are out or in the pipeline for all Industrial Innovation Areas (IIAs).

In the same fashion as previous years, the iCSI team had the opportunity to gather in an idyllic lake location for the Annual Seminar, this time Selbusjøen. Students, academics, researchers, industrial partners and scientific advisory committee members (52 participants) had the opportunity to spend two days together and exchange experiences, knowledge and ideas.

In addition, a workshop on “Challenges in Catalysis Research” was organized from iCSI, where students and industrial researchers working on catalysis had the opportunity to gather and discuss their challenges. The excellent talks from two industrial seniors on real-world catalysis puzzles that they have tackled during their career at Topsøe and Yara were the apogee of a purposely professor-free event with a lot of social interaction.

Three iCSI PhD candidates did industrial exchanges in 2018, to Herøya (Yara), Lillestrøm (Dynea)/Hamar (KA Rasmussen), and Lyngby (Haldor Topsøe). They returned noticeably wiser while also having contributed with new perspectives and skills at the industrial site.

Once more the representation at iCSI Board has changed. UiO representative Vebjørn Bakken changed role to become director of UiO: Energy. UiO is now represented by Kristin Vinje, Vice Dean at the Faculty of Mathematics and Natural Sciences at UiO. While Vebjørn made indispensable contributions in establishing the iCSI research and collaboration, Kristin brings new perspectives with her background from politics as well as research and innovation.

Finally, a big part of 2018 was devoted to preparations for the Midway evaluation that will be finalized in 2019. The administrative team was strengthened with experienced staff for tackling the reporting and coordination required. This exhaustive team effort is now almost complete, and we hope that we will have the opportunity to continue working in the fascinating world of industrial catalysis with impact to our societies for many years to come!

<https://www.ntnu.edu/icsi>



## Ph.D. Candidates and Postdoctoral Projects

### Insights into the kinetics and mechanism of selected industrial catalyzed reactions

**Ph.D. Candidate:** Moses Mawanga

**Supervisor:** Edd Anders Blekkan

**Co-supervisor:** Jia Yang

In heterogeneous catalysis, the study of the sequence of events occurring as reactant molecules are converted to products and the accompanying kinetics is sophisticated without an underlying proposed reaction mechanism in place. Knowledge of the kinetics and rate law that accurately describe the catalytic reaction helps to understand the controlling chemical reactions and thereby aid in selecting the reaction conditions that evoke the favorable reaction path over another, thus maximizing the desirable products.

The goal of the project is to conduct mechanistic and kinetic studies in the transient regimes to provide fundamental experimental data for some selected industrial catalyzed reactions. This approach will guarantee the qualitative and quantitative determination of the composition of adsorbed surface species during the reaction and provide information on the sequence of elementary steps that govern the global reaction kinetic rate. The project is comprised of two parts: Part I – which entails the investigation of intrinsic kinetics of the oxidation reaction of nitric oxide; a reaction that is fundamental to the Ostwald process. Supported platinum, manganese-based catalysts as well as perovskites will be tested to understand the structure–activity dependence of the catalytic system to understand the mechanism (Mars-van Krevelen/ Eley-Rideal/ Langmuir-Hinshelwood type) by which the catalyst functions in converting nitric oxide to dioxide. More so, the combined SSITKA-FTIR setup will also help to discriminate between the reactant species as well as spectator species on the catalyst surface. Part II – involve using the adsorption microcalorimetry to measure the heats of adsorption for catalytic activation and functionalization of light alkanes, e.g. using zeolites or copper-based catalysts. Heats of adsorption are indicative of the adsorption energetics and bonding strength of surface species to probe the nature of active sites of the catalyst. With these fundamental experimental data, it will be possible to have a better understanding of the catalytic reactions and thereby use the data for better catalyst design.

#### **Financial support:**

The project is a research activity (IIA6, WP6.3) under iCSI – Industrial Catalysis Science and Innovation for a competitive and sustainable process industry”, which is a National Centre for Research-based Innovation (SFI) granted by the Research Council of Norway.

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

**Ph.D. Candidate:** Eirik Østbye Pedersen

**Supervisors:** Prof. Edd A. Blekkan

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

Fischer-Tropsch synthesis (FTS) is mainly used for production of longer alkanes for fuel use and has been subject to thorough research throughout the 20<sup>th</sup> century. More recent research works show that high selectivity for light (C<sub>2</sub>-C<sub>4</sub>) 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 we have worked at obtaining a better understanding of chain growth and termination in the FTO process as a function of catalyst properties. The work has applied a multiscale approach, integrating first principles calculations (DFT), and advanced catalyst preparation, characterization and testing methods.

Manganese is considered an important promoter for increasing light olefin selectivity in the Fischer-Tropsch process. FTS over Mn-promoted Co/Al<sub>2</sub>O<sub>3</sub> catalysts is investigated by combining experimental and theoretical methods.

The effect of Mn promotion on Co catalysts is investigated by varying catalyst preparation method and reduction conditions. The state of Mn and its effect on Co is investigated using *in situ* characterization techniques such as XANES and XRPD under relevant reaction conditions and the role of Mn in H<sub>2</sub> and CO adsorption on Co will be investigated using SSITKA, and XPS.

The promotion effects of Mn on Co is also investigated by DFT. Calculations focus on the effect of Mn addition on the adsorption energies of relevant species on Co as well as the dissociation of CO, the formation of CH<sub>4</sub> and the formation and desorption of light olefins. The structure and promotion effect of MnO is studied, particularly the role of the Co-MnO interface.

### **Publications and reports in 2018:**

Østbye Pedersen, Erik: Mn promotion effects in Co based Fischer-Tropsch production of light olefins. Doctoral theses at NTNU, 2018:180. ISBN 978-82-471-4196-0

Østbye Pedersen, Eirik; Blekkan, Edd Anders: Noble Metal Promoted CoMn Catalysts for Fischer-Tropsch Synthesis. *Catalysis Letters* 148 (2018) 1027-1034.

Østbye Pedersen, Eirik; Svenum, Ingeborg-Helene; Blekkan, Edd Anders: Mn promoted Co catalysts for Fischer-Tropsch production of light olefins – An experimental and theoretical study. *Journal of Catalysis* 361 (2018) 23-32.

### **Presentations in 2018:**

Østbye Pedersen, Eirik; Svenum, Ingeborg-Helene; Blekkan, Edd Anders: Mn-promotion of alumina-supported cobalt Fischer-Tropsch catalysts. Oral presentation, 18th Nordic Symposium on Catalysis - NSC2018; Copenhagen, Denmark 2018-08-26 - 2018-08-28.

### **Financial support:**

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

## Chemical Looping Desulfurization

**PhD candidate:** Jianyu Ma

**Supervisors:** Prof. Edd A. Blekkan,

**Co-supervisor:** Research Scientist Kumar R. Rout, SINTEF.

Bioenergy is a significant contributor to the renewable energy supply in Norway, today mainly used for heating. Syngas from biomass gasification can be used for electricity production or chemical synthesis to produce synthetic fuels. The gas is a complex mixture including H<sub>2</sub>, CO, H<sub>2</sub>O, as well as S- containing species, which lead to the formation of H<sub>2</sub>S or other sulfides that can cause corrosion of downstream equipment and poison catalysts used for fuel synthesis. Hence, removal of sulphur is important for utilizing biomass on energy producing.

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

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

### **Publications and presentations in 2018:**

Blekkan, Edd Anders; Ma, Jianyu; Rout, Kumar Ranjan; Stavnes, Siri: Zirconium promoted manganese-based solid sorbents for H<sub>2</sub>S capture. 10th Int, Conference on Environmental Catalysis and 3rd EECAT; Tianjin, China 2018-09-22 - 2018-09-26.

Chytil, Svatopluk; Kure, Milly; Lødeng, Rune; Rout, Kumar Ranjan; Ma, Jianyu; Blekkan, Edd Anders: Supported manganese sorbents for H<sub>2</sub>S capture. 25th Int. Symposium on Chemical Reaction Engineering (ISCRE); Florence, Italy 2018-05-20 - 2018-05-23.

### **Financial support:**

Norwegian Research Council, project no. 267986



## Advanced biofuels via synthesis gas

**PhD candidate:** Ljubisa Gavrilovic

**Postdoc:** Qingjun Chen

**SINTEF:** Ingeborg-Helene Svenum.

**Supervisors:** Profs. Edd A. Blekkan, Hilde J. Venvik, Anders Holmen

In this project we have investigated some issues important for the development of second generation (2G) biofuels from biomass via gasification and fuel synthesis using the Fischer-Tropsch (FT) synthesis. The synthetic fuels are well suited as feedstocks for the production of diesel and aviation fuel (jet-fuel), and any kind of biomass can be used as feedstocks, including waste from agriculture or forestry industries. The process involves many steps, including pretreatment, gasification, gas cleaning and conditioning, the synthesis of hydrocarbons and product upgrading. Ash components, sulfur and other undesired elements in the biomass can form volatile species in the gasification step, and be transported with the gas and poison catalysts used in the process. We have studied several elements in this process. In order to improve the thermal efficiency of the process we have investigated hot gas cleaning, where solid sorbents play an important role. Our work on manganese-based solid sorbents for sulfur removal is continued in a new project, Chemical Looping Desulfurization. The effect of ash components on cobalt-based FT synthesis catalysts has been investigated both experimentally and theoretically. Potassium (K) was deposited on cobalt catalysts as aerosol particles, thus emulating the transport mechanism one can envisage in a gasifier. This work was done in close collaboration with the Linnaeus University in Växjö in Sweden. We have shown that even though the particles are deposited on the external surface of the catalyst, the effect is dramatic, indicating a high degree of mobility under the reaction conditions. Through theoretical calculations using DFT we have studied how minor coverages of potassium influence the adsorption and reaction on the cobalt surface. Also here is mobility an important point, and we have demonstrated very low barriers for surface diffusion of K atoms. K can then easily occupy important active sites on the surface, and in this way influence the surface reactions.

### Publications in 2018:

Ljubisa Gavrilovic: Fischer-Tropsch synthesis – Influence of aerosol-deposited potassium salts on activity and selectivity of Co-based catalysts. Doctoral thesis at NTNU, 2018:104 ISBN 978-82-326-2998-5.

Chen, Qingjun; Svenum, Ingeborg-Helene; Gavrilovic, Ljubisa; Chen, De; Blekkan, Edd Anders. Effect of trace potassium on hydrogen adsorption and dissociation on hcp cobalt: A density functional theory study. *Surface Science* 681 (2018) 24-31.

Gavrilovic, Ljubisa; Brandin, Jan; Holmen, Anders; Venvik, Hilde Johnsen; Myrstad, Rune; Blekkan, Edd Anders. Deactivation of Co-based Fischer-Tropsch Catalyst by Aerosol Deposition of Potassium Salts. *Industrial & Engineering Chemistry Research* 57 (2018) 1935-1942.

Gavrilovic, Ljubisa; Brandin, Jan; Holmen, Anders; Venvik, Hilde Johnsen; Myrstad, Rune; Blekkan, Edd Anders. Fischer-Tropsch synthesis—Investigation of the deactivation of a Co catalyst by exposure to aerosol particles of potassium salt. *Applied Catalysis B: Environmental* 230 (2018) 203-209.

Strømsheim, Marie Døvre; Svenum, Ingeborg-Helene; Farstad, Mari Helene; Li, Zheshen; Gavrilovic, Ljubisa; Guo, Xiaoyang; Lervold, Stine; Borg, Anne; Venvik, Hilde Johnsen. Effects of K adsorption on the CO-induced restructuring of Co(11-20). *Catalysis Today* 299 (2018) 37-46.

### **Presentations in 2018:**

Chytil, Svatopluk; Kure, Milly; Lødeng, Rune; Rout, Kumar Ranjan; Ma, Jianyu; Blekkan, Edd Anders. Supported manganese sorbents for H<sub>2</sub>S capture. 25th Int. Symposium on Chemical Reaction Engineering (ISCRE); Florence, Italy, 2018-05-20 - 2018-05-23.

Strømsheim, Marie Døvre; Farstad, Mari Helene; Svenum, Ingeborg-Helene; Gavrilovic, Ljubisa; Li, Zheshen; Guo, Xiaoyang; Lervold, Stine; Regli, Samuel K.; Borg, Anne; Venvik, Hilde Johnsen. Co(11-20) single crystal as Fischer-Tropsch catalyst model system. NorScatt Meeting; 2018-05-22 - 2018-05-22.

Strømsheim, Marie Døvre; Farstad, Mari Helene; Svenum, Ingeborg-Helene; Weststrate, C. J.; Gavrilovic, Ljubisa; Regli, Samuel K.; Li, Zheshen; Borg, Anne; Venvik, Hilde Johnsen. The effect of K on the adsorption and decomposition of ethylene on Co(11-20). Tailor2018: Tailored surfaces in operando conditions; 2018-06-11 - 2018-06-14.

### **Funding:**

The Research Council of Norway, contract no. 228741

## Bio-ethanol steam reforming for on board hydrogen generation system

**PhD. Candidate:** Mario Ernesto Casalegno  
**Researcher:** Dr. Nikolaos Tsakoumis  
**Supervisor:** Professor De Chen, Professor Edd A. Blekkan

The transition towards more sustainable means of energy production, distribution and use is a key issue. Slowing down, or even reversing the negative climatic effects from the utilization of fossil fuels is the ultimate goal. Utilization of hydrogen (H<sub>2</sub>) as an energy carrier can be a sustainable solution that will reduce the impact of human activities on the environment. Provided that H<sub>2</sub> is produced in a sustainable way from renewable sources, such as water (using renewable energy) or from biomass it has the potential, through its use in fuel cells with favorable efficiencies, to cover energy needs with a significant reduction in greenhouse gas emissions. H<sub>2</sub> production through steam reforming of hydrocarbons is a mature technology that can be extended to use ethanol as a feedstock. Bioethanol formed by fermentation processes has significant advantages and appears to be a strong candidate as an energy vector suitable for H<sub>2</sub> production.

Our efforts in this project are focusing on the creation of a prototype that integrates steam reforming of bioethanol for hydrogen production with hydrogen combustion into a compact multichannel reactor that can be used on board vehicles. Optimization of catalytic materials for both reaction applications will be assisted by kinetic experiments and theoretical calculations that will be used for building a microkinetic model. The optimal process conditions to run the experiments will be calculated using Aspen Plus simulator.

### Financial support:

Funding: NTNU TSO-Energy. Sino-Norwegian joint researcher projects NTNU – SJTU / Tsinghua University.

### *Other N. Tsakoumis activity in 2018:*

N.E. Tsakoumis, E. Patanou, S. Lögdberg, R.E. Johnsen, R. Myrstad, W. van Beek, E. Rytter, E.A. Blekkan, Structure-performance relationships on Co based Fischer – Tropsch synthesis catalysts: The more defect free the better, ACS Catal. 9 (2018) 511-520.

E. Rytter, Ø. Borg, N.E. Tsakoumis, A. Holmen, Water as key to activity and selectivity in Co Fischer-Tropsch synthesis:  $\gamma$ -alumina based structure-performance relationships, J. Catal. 365 (2018) 334–343.

E. Patanou, N.E. Tsakoumis, R. Myrstad, E.A. Blekkan, The impact of sequential H<sub>2</sub> -CO-H<sub>2</sub> activation treatment on the structure and performance of cobalt based catalysts for the Fischer-Tropsch synthesis, Appl. Catal. A Gen. 549 (2018) 280–288.

E. Rytter, A. ul R. Salman, N.E. Tsakoumis, R. Myrstad, J. Yang, S. Lögdberg, A. Holmen, M. Rønning, Hydrophobic catalyst support surfaces by silylation of  $\gamma$ -alumina for Co/Re Fischer-Tropsch synthesis, Catal. Today. 299 (2018) 20–27.

C. Sprung, E.A. Redekop, R.D. Armstrong, N.E. Tsakoumis, Midnight-sun-induced natural gas conversion, Catal. Today. 299 (2018) 2–9.

## Carbon Nanomaterial-Ionic Liquid Hybrid for Ultrahigh Energy Supercapacitor

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

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

To date, a maximum specific capacitance of 300 F/g using an operating voltage window of 4 V has been achieved in this work. Addition of TMABF<sub>4</sub>, TEABF<sub>4</sub> or smaller cations like Li<sup>+</sup>, Na<sup>+</sup>, Mg<sup>2+</sup> or Zn<sup>2+</sup> to the ionic liquid, could be a promising method to further enhance the capacitance. Achieving these goals would enable a wide application range in the energy sector and improve renewable energy storage and conversion. This project could promote the use of renewable energy in the public transportation sector.

### **Financial Support:**

The project is funded by the Research Council of Norway.

## Impact of promoters on ethylene oxychlorination catalyst

**Ph.D. candidate:** Hongfei Ma

**Supervisor:** Prof. De Chen

**Co-supervisor:** Res. sci. Kumar Ranjan Rout and ind.res. Terje Fuglerud

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

It has been reported that addition of  $MgCl_2$  does not affect the reducibility of the active phase of  $CuCl_2$  while KCl and CsCl addition decrease the reducibility because of the formation of the mixed salts of  $CuK_xCl_{2+x}$  and  $CuCs_xCl_{2+x}$ . [3] Revealed by the TPR profiles, all samples display a sharp peak around  $180^\circ C$ . The temperature at the peak position increase with K addition, indicating stronger Cl bonding with Cu or decreased the adsorption of ethylene. On the contrary, Mg addition to both Cu and promoted by K catalysts shifts the temperature peak position. The relation of reduction temperature peak versus Mg (or K) percentage (molar ratio of K or Mg in total molar of K and Mg) is shown in Figure 1. The higher the Mg content, the lower is the temperature peak position, while K behaves the opposite. In the impregnated catalysts, only  $Al_2O_3$  was visible in XRD patterns. Hence, dried ( $120^\circ C$ ) precipitates from equimolar, aqueous solutions of  $CuCl_2 \cdot 2H_2O$  and the respective KCl and  $MgCl_2 \cdot 6H_2O$  salt determined the presence of  $CuKCl_3$  and indicated  $Cu_3Mg(OH)_6Cl_2$ . A likely OH source in the latter is moisture adsorbed during analysis. While XRD analysis in a heated, dry atmosphere is planned at the ESRF beamline in April, it seems evident that K can be incorporated into the Cu lattice much more easily than Mg.

Based on our group's previous research, step transient and steady-state operando kinetic studies can provide the exact information of the transformation of Cu (II) and Cu (I). Also, by using in situ UV-Vis-NIR spectrometry, reaction rate and band gap information will obtain. Last, temperature programmed oxidation experiments are also under running; more information about the effect of promoter to the oxidation step will be added.

### Financial support:

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

### References:

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

**Ph.D. Candidate:** Martina Cazzolaro

**Supervisor:** Prof. De Chen

**Co-supervisor:** Assoc. Prof. Jia Yang

Various biomass-based processes lead to the production of hydroxyacetone (HA), i.e. biomass pyrolysis, sugar hydrogenolysis, glycerol dehydration. Via selective hydrogenation of HA, a major commodity chemical as 1,2-propanediol (PD) can be produced. Cu-based catalysts showed good activity in hydro-deoxygenation of bio-oil from biomass pyrolysis, but coke formation resulted in shortened catalyst lifetime. High activity was also observed in hydrogenolysis of glycerol to PD, having HA as dehydration intermediate: Cu particle size, dispersion and active area were reported to be of great importance for high activity and stability; particles agglomeration and formation of irregularly shaped clusters were suggested as deactivation causes. Carbon nanofibers (CNF) are attractive catalyst supports having high surface area and large number of edges, exploitable as metals anchoring sites. Moreover, surface oxidation, foreign-ion doping or confinement effect can be used to adjust CNF surface properties. This project aims to develop a stable Cu-based catalyst for selective gas-phase hydrogenation of HA to PD, by tuning the carbon support properties.

Platelet carbon nanofibers were prepared via CVD of CO and H<sub>2</sub> at 600°C over Fe powdered nanoparticles and were characterized with TGA, N<sub>2</sub> physisorption, H<sub>2</sub>-TPR and TEM. 9 catalysts with 5wt% Cu loading were prepared via IWI of PCNF with 3 Cu precursors (nitrate, acetate and basic carbonate) and 3 solvents (water, ethanol, propanol). The catalysts were analyzed with TGA, N<sub>2</sub> physisorption and H<sub>2</sub>-TPR. Non-carbonaceous reference catalysts supported over silica were tested in HA hydrogenation to PD, showing good activity (conversion and selectivity up to around 80%). 21% yield loss was observed over a test of 48 hours indicating deactivation. Activity tests and characterization of PCNF-supported catalysts will follow. Surface treatment of CNF will be explored.

### Poster presentation in 2018:

Martina Cazzolaro, Jia Yang, Jørgen Svendby, Rik de Clercq, Irantzu Sadaba Zubiri, Esben Taarning, De Chen. *Selective hydrogenation of hydroxyacetone to 1,2-propanediol – catalyst development.*

Bio4Fuels Days 2018. Oslo, Norway.

iCSI Seminar 2018. Selbusjøen, Norway.

### Financial support:

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

## Promoter Effects on Ethylene oxychlorination reaction for CuCl<sub>2</sub>/γ-Al<sub>2</sub>O<sub>3</sub> based catalysts

**Ph.D. candidate:** Endre Fenes

**Supervisor:** Prof. De Chen

**Co-supervisor:** Industry researcher 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<sub>2</sub>/γ-Al<sub>2</sub>O<sub>3</sub> based catalysts and consists of three distinct reaction steps in which copper cycles between Cu<sup>2+</sup> and Cu<sup>1+</sup> oxidation states: catalyst reduction by ethylene, consuming chlorine from the catalyst, catalyst oxidation and at last, catalyst hydrochlorination.

In this project, the effect of promoters, i.e., mostly alkali, alkali earth and lanthanide elements on turnover frequency, catalytic activity, selectivity and stability is investigated with an operando study, combining mass- and UV-Vis-NIR spectrometry during both transient and steady state experiments. We developed a kinetic model based on our experimental data and DFT calculations by dr. Yanying Qi and we are now in the process of publishing the results.

Last year our work gathered international attention, and in February, we adapted our experimental approach to NO<sub>x</sub> abatement catalysis in cooperation with researchers from Politecnico de Milano and a joint publication is currently submitted. In addition, the work was presented by De Chen as a keynote lecture at ISCRE 25 in Florence and as an oral presentation at the Nordic catalysis symposium.

In April, we travelled to the Swiss-Norwegian beamline at ESRF in Grenoble to combine operando UV-Vis and X-ray absorption spectroscopy. The effort resulted in large data sets which we are still processing. Coordinating all these efforts have taken more time than expected and I am a little bit behind schedule with my Ph.D. On the positive side, cooperating with several researchers have been highly interesting and I am optimistic it will pay off in the end.

### Publications 2018:

M. F. Baidoo, E. Fenes, K. R. Rout, T. Fuglerud, D. Chen: On the effects of K and La co-promotion on CuCl<sub>2</sub>/γ-Al<sub>2</sub>O<sub>3</sub> catalysts for the oxychlorination of ethylene. *Catalysis Today*, 2018, 299. 164-171

W. Hu, T. Selleri, F. Gramigni, E. Fenes, K. R. Rout, I. Nova, E. Tronconi, X. Gao, D. Chen, K. Cen A HONO-based mechanism for the reduction half-cycle in the low temperature Selective Catalytic Reduction of NO over Cu-CHA, *Applied Catalysis B: Environmental* 2019 (submitted)

### Presentations 2018:

Fenes E., Rout K.R., Baidoo M., Fu W., Duan X., Chen D., Fuglerud T. Descriptors for alkali metal promotion in redox catalysis: ethylene oxychlorination, (poster) ISCRE 25, Florence 2018.

De Chen, kinetic analysis and design of catalytic redox cycles, (keynote) ISCRE 25, Florence 2018.

Fenes E., Ma H., Rout K.R., Chen D., Fuglerud T. Calcined Al-Mg Hydrotalcite as Support in CuCl<sub>2</sub> Based Oxochlorination Catalysts. 18th NSC, Copenhagen 2018.

**Financial support:**

Industrial Catalysis Science and Innovation (iCSI)



## **Kinetic Study of Bimetallic Catalysts for Compact Steam Reformer**

**Ph.D. Candidate:** Shirley Elisabeth Liland  
**Supervisor:** Prof. De Chen  
**Co-supervisor:** Research Scientist 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).

For both reactions several Ni-Co based catalysts supported on a hydrotalcite-structure has been studied. For the SR reaction it has been found that the bimetallic Ni-Co catalyst severely enhances the activity compared to pure Ni and pure Co. The same catalysts have also been investigated for the total combustion reaction, as this reaction is also relevant for methane decomposition. Here it was found that Co is the most active, and that promoting it with Pd enhances the activity further. During the total combustion reaction experiment a UV-vis-NIR spectroscopy was utilized together with a GC and a MS, making it an operando set-up which relates the oxidation state of the active metals with the activity and selectivity. The reason for the difference in both activity and selectivity for Ni and Co is believed to be difference in reaction mechanisms, where Ni is partly or fully influenced by the Mars-Van Krevelen mechanism while Co is reacting by the Langmuir-Hinshelwood mechanism. In the period August 2017 to June 2018, Najma Ali Abdullahi, wrote her master thesis on catalytic combustion using the same setup.

The end goal for this project is to collect information and to increase our knowledge which will lead to more attractive investments in industrial processing of natural gas in Norway.

### **Publications and presentations in 2018**

Liland, Shirley Elisabeth; Rout, Kumar Ranjan; Fenes, Endre; Yang, Jia; Chen, De. Rational Design of Ni-Co/Hydrotalcite Catalyst for Methane Total Combustion. 25th International Conference on Chemical Reaction Engineering; May 20-23, 2018, Florence, Italy. Poster

Liland, Shirley Elisabeth; Rout, Kumar Ranjan; Chen, De, Operando study: Oxidation of Ni-Co/HT Catalyst for Catalytic Combustion of Methane. Nordic Symposium on Catalysis. August 26-28, 2018, Copenhagen, Denmark. Oral Presentation

Niu, Juntian; Liland, Shirley Elisabeth; Yang, Jia; Rout, Kumar Ranjan; Ran, Jingyu; Chen, De. Effect of oxide additives on the hydrotalcite derived Ni catalysts for CO<sub>2</sub> reforming of methane. Chemical Engineering Journal. 2018.

**Financial support:**

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

## **Integrated H2BioOil Process for Efficient Biofuel Production**

**PhD. Candidate:** Isaac Yeboah

**Supervisor:** Prof. De Chen

**Co-supervisor:** Dr. Kumar Ranjan Rout

The interest for renewable energy sources has increased over the decades due to the over reliance on fossil fuel for transport fuel. Although, there are several paths to convert solid biomass chips to fuel, to date no sustainable route has matured. Bio-oil produced from pyrolysis seem promising route towards sustainable biorefinery concept. In this project, biofuel is prepared from the integration of fast-hydropyrolysis (FHP) and tandem catalytic packed bed reactors. The bio vapors generated from FHP reactor is upgraded in catalytic reactor, having carbon coupling and hydrodeoxygenation (HDO) catalyst. The HDO catalyst is designed using modified Pichini method with Ru as promoter and MoXP (X: Ni, Fe, Co, Ru etc.) as an active phase on commercial Al<sub>2</sub>O<sub>3</sub> pellets support. Comprehensive catalyst characterization techniques such as HRTEM/EDS, TPD, XPS, TGA, BET, and XRD etc. were employed to reveal physicochemical properties of the catalyst. The reaction product identification and quantification (conversion, yield and selectivity) were done in a multi-purpose installed GC-FID, GC-MS (NIST11 library), and HPLC-MS. Our preliminary findings revealed a well dispersed 1 wt % Ru promoted bimetallic phosphide (20 wt MoFeP) catalyst supported on alumina spheres (4 mm). The promoted Ru clustered catalyst showed higher Lewis Acid Site /Brønsted Acid Site ratio and exhibited remarkable selectivity to C-O phenolic bonds cleavage towards high yield (ca. 70%) jet fuel range hydrocarbon production using simulated bio oil feedstock. A significant hydrodeoxygenation degree was observed for the Ru promoted catalyst. The findings and the understanding will be relevant for the conversion of wood chips to fuel.

### **Patent Filed**

De Chen, Kuman R. Rout, Isaac Yeboah, 'Preparation of Biofuel from Biomass', Jan.2019, United Kingdom (UK), Patent Application No. 19005537.

### **Conference presentations 2018:**

Yeboah, Isaac; Xiang Feng, Kumar R., Rout; De, Chen. Simultaneously enhanced yield and purity of aviation fuel derived from biomass-derived light oxygenates by one-pot cascade reactions. The 10th International Conference on Environmental Catalysis & the 3rd International Symposium on Catalytic Science and Technology in Sustainable energy and Environment; (ICEC&EECAT), 2018-09-22 - 2018-09-26, Tianjin, China. Oral

Yeboah, Isaac; Kumar R., Rout; Xiang Feng, G. Fan, C. Van der Wijst; Suizhong Li ; De, Chen. Insight into Catalytic In-Situ Co/Pyrolysis of Biomass Powder and Bio-Oil as Hydrogen Donor to Green Aromatics, 26TH European Biomass Conference & Exhibition, EUBCE; 2018-05-14 - 2018-05-17, Copenhagen, Denmark. Oral

Yeboah, Isaac; G. Fan; Kumar R., Rout; Jia Yang; De, Chen. Insight into Catalytic In situ Co-pyrolysis of Pine and Heavy fraction of Bio oil using PyGCMS, Norwegian Catalysis Symposium, NKS; 2017-11-06 - 2017-11-07, Oslo, Norway. Oral.

## **Model-aided catalyst prediction through descriptor-based hybrid semi-empirical approach**

**PhD candidate:** Yalan Wang

**Supervisor:** Professor De Chen

Microkinetic model aided catalyst prediction is an advanced method for developing improved and novel catalysts without intensive empirical testing in heterogeneous catalysis. The model offers the possibility to help understand reaction mechanism and aid rational catalyst design. Currently, density functional theory (DFT) calculation is the most popular method to estimate input parameters of microkinetic model with high accuracy. However, DFT calculations normally spend overmuch time and are computationally expensive. As such, a descriptor-based hybrid semi-empirical approach (UBI-QEP + BEP) is advocated here to rapidly acquire energetics for transition metal surface reactions. In this approach, adsorption energies are estimated by the improved UBI-QEP method, which is modified according to DFT values, with only atomic binding energies as descriptors. BEP relationships fitted from DFT data are utilized to calculate activation energies. The obtained energetics are subsequently applied in CatMAP to conduct microkinetic modeling and generate reaction rate volcano, based on that to do catalyst screening and design. A preliminary microkinetic modeling of steam methane reforming (SMR) demonstrates that the approach displays reasonable accuracy with respect to DFT computations as well as experiments, but reduces radically six orders of magnitude in the computational expenses.

Size-dependent activity of SMR is studied on Rh, Ni, Pt and Pd catalysts by using microkinetic modeling combined with a truncated octahedron model, which illustrates the higher activity on the smaller sized metal particles. Substantially higher activity of M(211) than M(111) and M(100) accompanied by decreased M(211) surface fraction results in reduced metal activity as the particle size increases. The metal-dependent mechanism of Fischer-Tropsch synthesis (FTS) indicates that CO insertion is the main mechanism for FT reaction. CO activation occurs primarily via H-assisted CO dissociation. The major C1/ C2 chain growth take place through CH + CO/ CH<sub>3</sub>C + CO coupling. Ni<sub>3</sub>Cu and Ni<sub>3</sub>Zn are suggested as potential bimetallic catalysts for FTO (Fischer-Tropsch to Olefins) through screening of large amounts of A3B type bimetallic catalysts, which show both high activity and economic advantage. This work offers a feasible approach to gain insight into the size-dependent and metal-dependent activity as well as mechanism, further to aid rational catalyst design in heterogeneous nanocatalysis.

### **Publications in 2018:**

Y. Wang, X. Wang, Y. Zhu, K. Zhu, D. Chen, X. Zhou, Shape Selectivity in Acidic Zeolite Catalyzed 2-pentene Skeletal Isomerization from First Principles, *Catalysis Today* (In Press), 2018.

### **Presentations in 2018**

Y. Wang, L. Xiao, Y. Qi, Y. Zhu, J. Yang, W. Xiao, D. Chen, A. Holmen, Model-aided catalyst prediction for H<sub>2</sub> production from steam reforming through hybrid semi-empirical approach. Oral presentation. The 10th International Conference on Environmental Catalysis &

the 3rd International Symposium on Catalytic Science and Technology in Sustainable Energy and Environment, Tianjin, China. September 22-26, 2018.

**Financial support:**

This project is financed by NTNU.

## Catalysts for NO<sub>x</sub>-reduction in maritime transportation

**Ph.D. Candidate:** Ole Håvik Bjørkedal

**Supervisor:** Prof. Magnus Rønning

**Co-supervisor:** Senior Researcher Rune Lødeng

Stricter regulations for maritime nitrogen oxide (NO<sub>x</sub>) emissions are expected to create a demand for non-toxic NO<sub>x</sub>-reduction catalysts able to perform at a wide range of operating conditions with special regards to oxygen content and temperature in the exhaust stream.

Liquefied Natural Gas (LNG) is becoming more attractive as maritime fuel, due to its increasing supply and opportunity for more efficient and cleaner combustion. However, the combustion process is usually performed with surplus oxygen to minimize the risk of methane slip. Such conditions facilitate generation of thermal NO<sub>x</sub>, which must be reduced downstream of the engine.

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

High surface area, surface acidity and thermal stability are regarded to be important properties for an SCR-catalyst. Mesoporous alumina (MA) prepared through a sol-gel synthesis may be a way to obtain these properties in a support material. Catalysts with Fe and Cu on an MA-support have been synthesized and characterized. In-situ XAS/XRD experiments have been performed at the Swiss-Norwegian Beamline (SNBL) at ESRF in Grenoble to determine the state of the active metal during the SCR-reaction.

The current focus of the project is catalysts synthesized through a one-pot sol-gel method which should allow for a high metal (Cu or Fe) content that is highly dispersed on the surface. Performance and kinetic tests are in progress on a test rig that was recently commissioned.

A student, Lisa Leganger Landfald has joined the project for her master thesis. She is working with iron-zeolites and zeotypes (Fe-ZSM-5, Fe-SAPO 34), investigating synthesis methods and their influence on SCR performance.

### **Presentations in 2018:**

Bjørkedal, Ole Håvik; Rønning, Magnus. One-step sol-gel synthesis of Cu/Ordered Mesoporous Alumina. Norsk katalysesymposium; 2018-10-16 - 2018-10-17

Bjørkedal, Ole Håvik; Rønning, Magnus. One-step sol-gel synthesis of highly dispersed Cu/Ordered Mesoporous Alumina. iCSI Annual Seminar; 2018-11-19 - 2018-11-20

### **Financial support:**

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

## Nanostructured Hybrid Catalysts for Photocatalytic Applications

**Ph.D. Candidate:** Jibin Antony

**Supervisor:** Prof. Magnus Rønning

**Co-supervisors:** Ass. Prof. Jia Yang and Post Doc. Sulalit Bandyopadhyay

Ammonia is one of the most essential chemicals for the industrial production of fertilizers, pharmaceuticals, and several other nitrogenous compounds 1. The synthesis of ammonia requires high temperatures (400–600°C) and high pressures (20–40MPa), which leads to an annual consumption of around 1-2% of the world's energy supply, resulting in massive emission of greenhouse gases. The extreme energy demand required for the industrial production of ammonia along with depleting fossil fuels calls for the pressing need for an alternative greener synthesis route. Bismutite ( $\text{Bi}_2\text{O}_2\text{CO}_3$ ) has recently emerged as an important candidate in photocatalysis of ammonia 1. Controlling the size and shape of bismutite nanoparticles (NPs) has been reported to have significant effects on its activity 2. On the other hand, gold (Au) nanoparticles due to their excellent optical properties and localized surface plasmon resonance (LSPR) effect have been reported to significantly enhance solar energy collection efficiency of semiconductors 1,3. This project aims at synthesizing Au NPs using bottom-up approach and obtaining hybrid catalysts of these with semiconductor NPs and characterizing these catalysts using techniques such as UV-Vis, S(T)EM, BET, XRD, XPS and DLS. Finally, the catalytic activity of these hybrids would be analysed in a photoreactor setup, which is equipped with UV-Vis lamps and an additional solar simulator. The catalyst, which is in a suspension with water-alcohol solution, will be saturated with  $\text{N}_2$  by continuous purging. Nanostructured hybrids of Au NPs with bismutite and other semiconductors of interest synthesized, which when coupled with their morphological properties, is anticipated to pave way for energy efficient photosynthesis of ammonia.

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2. Zhang, X. et al. Controlled morphogenesis and self-assembly of bismutite nanocrystals into three-dimensional nanostructures and their applications. 2, 2275-2282 (2014).
3. Li, Q., Hao, X., Guo, X., Dong, F. & Zhang, Y. J. D. T. Controlled deposition of Au on  $(\text{BiO})_2\text{CO}_3$  microspheres: the size and content of Au nanoparticles matter. 44, 8805-8811 (2015).

### Financial support:

The project is funded by Department of Chemical Engineering, Norwegian University of Science and Technology (NTNU).

## Advanced in situ characterization of heterogeneous catalysts for sustainable process industries

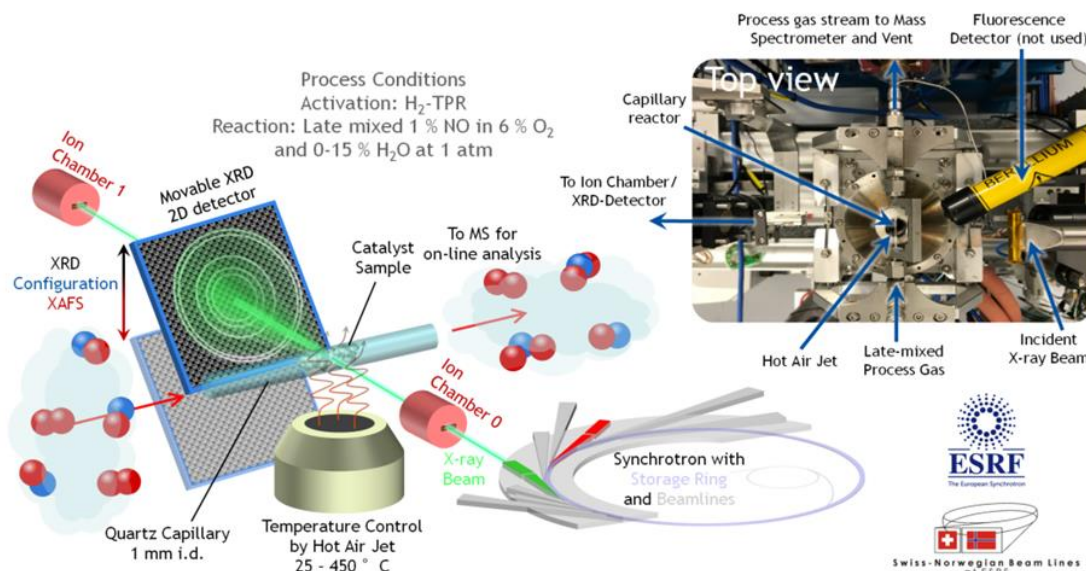
**PhD-candidate:** Samuel K. Regli

**Supervisor:** Prof. Magnus Rønning

**Co-Supervisor:** Prof. Hilde J. Venvik

This PhD project is part of the industrial Catalysis Science and Innovation (iCSI) Center. We are investigating heterogeneous catalysts during operation at industrially relevant conditions and develop the necessary data analysis tools as needed. In order to link structural properties of the material with catalytic activity during reaction, we apply spectroscopy (Infrared, X-ray, UV-Vis) in-house and at synchrotrons. We have synergies with four out of the six work packages within iCSI and collaborations within KinCat (Fe-based Fischer-Tropsch synthesis to olefins from renewable feedstocks and selective catalytic reduction of NO by ammonia over Cu-based catalysts), but also with SUNCAT in Stanford (Hydrogenation of CO and CO<sub>2</sub> to Methanol).

With our setup shown in the figure below, we can combine several techniques for simultaneous characterization of the bulk and the surface of catalysts during reaction at industrially relevant concentrations, temperatures (473-723 K) and pressures (up to 20 bar). Key characterization techniques in this project are X-ray absorption spectroscopy with synchrotron radiation, X-ray diffraction, UV-Vis spectroscopy, Fourier-transform infrared spectroscopy and Raman spectroscopy. New insight on the active sites of the catalysts and the respective kinetics of the chemical reactions can guide towards favorable compositions and conditions, thereby enabling processes with higher efficiency, lower cost, reduced emissions or by-products and improved lifetime.



**Figure:** Experimental Setup for combined operando powder X-ray diffraction and X-ray absorption spectroscopy with simultaneous product gas analysis by mass spectrometer at the Swiss Norwegian Beamlines BM31 at the European Synchrotron Radiation Facility, Grenoble, France



**Poster presentations in 2018:**

Regli SK, Salman AuR, Rønning M. In situ study of NO oxidation over Pt-based catalysts for nitric acid production. 6th International Congress on Operando Spectroscopy in Estepona, Málaga, Spain, April 2018.

Regli SK, Rønning M. Operando XRD and XAS study of nitric oxide oxidation over supported Pt catalysts. XAFS2018. Kraków, Poland, July 2018.

**Financial Support:**

This work is part of the industrial Catalysis Science and Innovation Centre for a competitive and sustainable process industry, which receives financial support from the Research Council of Norway under contract no. 237922.

## Catalysts for attaining NO/NO<sub>2</sub> equilibrium

**Ph.D. Candidate:** Ata ul Rauf Salman

**Supervisor:** Prof. Magnus Rønning,

**Co-supervisors:** Senior Scientists Rune Lødeng and Bjørn Christian Enger

Nitric acid is commercially produced via the Ostwald process. A key chemical step in the process is the oxidation of nitric oxide into nitrogen dioxide, which occurs as a homogeneous gas phase reaction requiring removal of heat and long residence time. The aim of the project is to replace the homogeneous process with a heterogeneously catalyzed process coupled with heat exchangers, permitting significant intensification of the nitric acid plant. Multiple advantages can be achieved by the use of a catalyst a) the oxidation process will be accelerated b) reduction in capital costs and c) additional heat recovery.

Replicating the demanding conditions of industrial NO oxidation in a laboratory reactor is challenging. Therefore, researchers at NTNU, SINTEF, and YARA AS collaborate to address this demanding research.

Catalytic oxidation of nitric oxide over supported platinum catalysts under industrial conditions have been investigated. Summarized results from the kinetics over Pt/Al<sub>2</sub>O<sub>3</sub> including reaction order, apparent activation energy, and proposed reaction mechanism were published in 2018. For an in-depth understanding of the evolution of chemical and structural changes of platinum nanoparticles during oxidation of NO, operando XAS and XRD experiments were performed at the European Synchrotron Radiation Facility (ESRF) in Grenoble, France.

Another major focus of the project is to identify potential replacement of PGM catalysts, exhibiting superior or comparable catalytic activity. Therefore, several transition metal oxides on different support material and perovskites have been investigated. The results are very promising and currently under finalization process.

### **Presentations / Publications in 2018:**

Salman, A.u.R.; Enger, B.C.; Auvray, X.; Lødeng, R.; Menon, M.; Waller, D.; Rønning, M. Catalytic oxidation of NO to NO<sub>2</sub> for nitric acid production over a Pt/Al<sub>2</sub>O<sub>3</sub> catalyst. *Applied Catalysis A: General* 2018, 564, 142-146.

Salman A.U.R., Enger B.C., Lødeng R., Menon M., Waller D., Rønning M. Catalytic oxidation of NO to NO<sub>2</sub> for nitric acid production over a supported Pt catalyst. 18<sup>th</sup> Nordic Symposium on Catalysis (NSC). August 26-28, 2018 Copenhagen Denmark, Presentation.

Salman A.U.R., Enger B.C., Lødeng R., Menon M., Waller D., Rønning M. A kinetic study of NO oxidation on Pt/Al<sub>2</sub>O<sub>3</sub> at conditions relevant to industrial nitric acid production. 25<sup>th</sup> International Conference on Chemical Reaction Engineering (ISCRE25) May 20-23, 2018 Florence Italy, Poster.

### **Financial support:**

This project forms a part of the iCSI (industrial Catalysis Science and Innovation) Centre for Research-based Innovation, which receives financial support from the Research Council of Norway under contract no. 237922.

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

**Ph.D. Candidate:** Stine Lervold

**Supervisor:** Prof. Hilde J. Venvik

**Co-supervisors:** Assoc. Professor Jia Yang and Senior Researcher Dr.ing Rune Lødeng (SINTEF).

Formaldehyde is the essential component of wood adhesives for a wide range of applications and an important intermediate in the production of several fine chemicals. Formaldehyde is produced via selective catalytic oxidation of methanol to formaldehyde. Industrially, production of formaldehyde from methanol is performed via two main processes: either partial oxidation over a silver catalyst or oxidation in excess air over base metal oxides. Dynea owns both technologies and recognizes an economic potential for the silver-based process with the main objective to improve the yield and lifetime of the silver catalyst. The PhD project focuses on kinetic experiments that can be linked to the surface structure and composition of the Ag catalyst. Initial activities have concerned the development of experimental protocols that allow extraction of kinetic data in the experimental setup, including specific reactor designs.

Electrolytic silver particles were studied in relation to its morphology changes under different reactive and non-reactive atmospheres, and its catalytic activity in oxidation of methanol to formaldehyde (MTF), carbon monoxide to carbon dioxide, and hydrogen to water. Scanning electron microscopy and X-ray diffraction (XRD) were applied to analyze structural changes in the silver catalyst after exposure or interaction with nitrogen, oxygen, methanol/water, carbon monoxide and hydrogen, applied either individually or in selected combinations, at temperatures approaching 700 °C. The as-received Ag catalyst consists of agglomerated, faceted, polycrystalline particles. Massive morphological changes occur during MTF reaction conditions, and similar severe restructuring on the mesoscopic scale with pinhole formation under oxygen containing atmospheres (O<sub>2</sub>/N<sub>2</sub>, H<sub>2</sub>/O<sub>2</sub>/N<sub>2</sub> and CO/O<sub>2</sub>/N<sub>2</sub>) at elevated temperature. For the CO and H<sub>2</sub> oxidation sub-systems, the initial activity was comparable. But, while the conversion of H<sub>2</sub> is preserved during time on stream, the CO conversion gradually reduces. This suggests that the restructuring associated with dissolution of O at high temperature inhibits the CO to CO<sub>2</sub> pathway.

### **Publications 2018:**

Stine Lervold, Kamilla Arnesen, Nikolas Beck, Rune Lødeng, Jia Yang, Kristin Bingen, Johan Skjelstad, Hilde J. Venvik. Morphology and Activity of Electrolytic Silver Catalyst for Partial Oxidation of Methanol to Formaldehyde Under Different Exposures and Oxidation Reactions. *Topics in Catalysis*, in print (<https://doi.org/10.1007/s11244-019-01159-0>).

### **Presentations in 2018:**

Stine Lervold, Kamilla Arnesen, Nikolas Beck, Rune Lødeng, Jia Yang, Kristin Bingen, Johan Skjelstad, Hilde J. Venvik. Morphology study of electrolytic silver catalyst for partial oxidation of methanol to formaldehyde (MTF). 8th Nordic Symposium on Catalysis (NSC), Copenhagen, Denmark, 2018. Poster presentation.

Stine Lervold, Kamilla Arnesen, Nikolas Beck, Rune Lødeng, Jia Yang, Kristin Bingen, Johan Skjelstad, Hilde J. Venvik. Morphology study of electrolytic silver catalyst for partial oxidation of methanol to formaldehyde (MTF). iCSI Annual Seminar, Selbusjøen, Norway, 2018. Poster presentation.

Stine Lervold, Kamilla Arnesen, Nikolas Beck, Rune Lødeng, Jia Yang, Kristin Bingen, Johan Skjelstad, Hilde J. Venvik. Morphology study of electrolytic silver catalyst for partial oxidation of methanol to formaldehyde (MTF). IKP-day NTNU, Trondheim, Norway, 2018. Poster presentation.

Stine Lervold, Kamilla Arnesen, Nikolas Beck, Rune Lødeng, Jia Yang, Kristin Bingen, Johan Skjelstad, Hilde J. Venvik. Investigations of the methanol to formaldehyde (MTF) reaction over silver. Challenges in Catalysis – iCSI workshop, Langesund, Norway, 2018. Oral presentation.

#### **Awards:**

Best Poster Award for her work on "Morphology study of electrolytic silver catalyst for partial oxidation of methanol to formaldehyde (MTF)" at the 18th Nordic Symposium on Catalysis in Copenhagen, from 26-28 August.

#### **Financial support:**

The project is a research activity (IIA3, WP3.1) under iCSI – industrial Catalysis Science and Innovation for a competitive and sustainable process industry”, which is a National Centre for Research-based Innovation (SFI) granted by the Research Council of Norway.

## **Material degradation by metal dusting corrosion in compact reformer concepts**

**Ph.D. Candidate:** Xiaoyang Guo

**Supervisor:** Prof. Hilde Johnsen Venvik

**Co-supervisors:** Prof. De Chen, Senior Scientist John Walmsley, Senior Scientist Per Erik Vullum and Dr. Estelle Vanhaecke

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

Ni and Fe - main constituents of industrial alloys applied at high temperature - are excellent catalysts for carbon formation. Alloys based on Ni and Fe are therefore susceptible to metal dusting corrosion, which becomes a costly issue for industrial process equipment applied in carbon-saturated gaseous environments such as that of synthesis gas manufacture. The overall objective of this work is to provide better understanding and prediction of the carbon formation phenomena leading to metal dusting, as well as enabling alloy selection and alloy pre-treatment procedures that minimize metal dusting corrosion.

Systematically pretreated Ni-based industrial alloy samples (INCONEL® 601) were subjected to metal dusting conditions as a function of time, composition and pressure at 750°C in order to capture the initial carbon formation. Investigations before and after carburizing gas exposure were performed by optical microscopy, SEM, AES and Raman spectroscopy. Dual-beam FIB-SEM was used to collect and prepare thin lamellas from site specific locations at the alloy surface for further advanced characterization by TEM.

The carbon deposition is clearly a function of the gas composition during exposure, less carbon is formed under 10% CO in Ar with infinite carbon activity than under synthesis gas with finite low carbon activity, which point to the impact of the reaction mechanism and kinetics. The characterization indicates that the metal dusting corrosion rate is lowered when Cr<sub>2</sub>O<sub>3</sub> rather than (Ni, Fe, Cr)<sub>3</sub>O<sub>4</sub> spinel is the major phase of the oxide scale. Fine-grain structure on the alloy surface is also found beneficial to the metal dusting corrosion resistance.

### **Publication in 2018:**

Xiaoyang Guo; Estelle Vanhaecke; Jianyu Ma; P.V.D.S. Gunawardana; John C. Walmsley; De Chen and Hilde J. Venvik. Effects of metal dusting relevant exposures of alloy 601 surfaces on carbon formation and oxide development. To be submitted.

### **Financial support:**

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

Yeboah, Isaac; Kumar R., Rout; Xuezhi, Duan; De, Chen. A tandem aldol and hydro deoxygenation (HDO) reactions of Bio-Oil oxygenates fraction to hydrocarbon. NAM2017; 2017-06-04 - 2017-06-11, Denver, USA. Oral.

van der Wijs, Cornelis Gerardus; Rui, Haakon Marius Vatten; Yeboah, Isaac; Duan, Xuzhi.; Kovačič, Dávid; Liland, Ingvil Skeie; Chen, De. Synthesis and applications of multifunctional carbon-based catalysts for cellulose conversion. CarboCat VII; 2016-06-12 - 2016-06-17, Strasbourg, France. Oral.

Yeboah, Isaac; Kumar Ranjan Rout; and De Chen, Tandem catalytic upgrading of simulated bio oil to Jet fuel range aromatics: effects of upstream catalyst. iCSI Seminar, Nov-20-21, 2018, Selbu, Trondheim, Norway. Poster

Yeboah, Isaac; Kumar R., Rout; Jia Yang; De, Chen. Valorization of light Oxygenates in Bio-Oil via Catalytic Tandem reaction involving C-C bond Formation, European Biomass Conference and Exhibition, EUBCE; 2018-05-14 - 2018-05-17, Copenhagen, Denmark. Poster.

**Financial support:**

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

## **Enhanced visible light adsorption TiO<sub>2</sub> based catalysts for photocatalytic H<sub>2</sub> production**

**Ph.D. Candidate:** Muhammad Zubair

**Supervisor:** Assoc. Prof. Jia Yang

**Co-Supervisor:** Prof. Magnus Rønning

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

Titanium dioxide (TiO<sub>2</sub>) is n-type ideal semiconductor photo catalyst, which is being widely used in H<sub>2</sub> production, environmental purification, self-cleaning, CO<sub>2</sub> reduction, organic synthesis and solar cells due to high thermal stability, cost-effective, nontoxic and environmentally friendly. Due to the wide band gap (3.2 eV) of TiO<sub>2</sub>, it can only absorb UV light up to 380 nm, which is an intrinsic limitation for the TiO<sub>2</sub>-based photo catalyst to efficient light harvesting. The charge separation efficiency is a crucial factor for the efficient photocatalytic activity of TiO<sub>2</sub>. In spite of its versatility, the mobility of electrons in TiO<sub>2</sub> is low which affects the electron transport rate leading to a decrease in the collection efficiency of the photo generated electrons. Numerous TiO<sub>2</sub> based photo catalyst have developed for half photocatalytic reaction for H<sub>2</sub> by using the sacrificial reagents by utilizing the photo generated electrons in the conduction band. These inorganic sacrificial reagents can be easily oxidized to produce different harmful products by the photo generated holes and promote the H<sub>2</sub> production reaction and making the photocatalytic system expensive. Till the time, there is no such catalysts available with a state of the art efficiency, selectivity and stability along with the efficient and ideal photo reduction setup.

In this project, to overcome the above-mentioned problem, various approaches like heterojunction formation of TiO<sub>2</sub> with narrow band gap semiconductor, doping of heteroatom, application of co-catalysts will be applied to increase the photocatalytic activity of semiconductor materials (TiO<sub>2</sub>) which are thermally stable, abundance, cost effective and biocompatibility.

### **Publications:**

M. Zubair, I.-H. Svenum, M. Rønning, J. Yang, *Catal. Today.* (2018). doi:10.1016/j.cattod.2018.10.070

**Oral Presentations:**

Facile synthesis approach for core-shell TiO<sub>2</sub>-CdS nanoparticles for enhanced photocatalytic H<sub>2</sub> generation from water, Norwegian Catalysis Symposium, October 16th and 17th 2018, Lillestrøm, Norway

Photocatalysis for renewable energy conversion: A brief introduction and application of different semiconductor materials for production of H<sub>2</sub> from water, IKP Dagen 2018, Chemical engineering department, NTNU, Trondheim, Norway

**Poster Presentations:**

Facile synthesis approach for core-shell TiO<sub>2</sub>-CdS nanoparticles for enhanced photocatalytic H<sub>2</sub> generation from water, 10th European meeting on Solar Chemistry and Photocatalysis: Environmental Applications (SPEA10), 4-8 June 2018. Almería, Spain

Facile synthesis approach for core-shell TiO<sub>2</sub>-CdS nanoparticles for enhanced photocatalytic H<sub>2</sub> generation from water, NTNU Nano-Lab symposium, 28-29 Nov 2018, Trondheim, Norway

**Financial support:**

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



## **Novel Fe catalysts for the Fischer Tropsch synthesis based on renewable feedstocks**

**Ph.D. Candidate:** Joakim Tafjord

**Supervisor:** Ass. Prof. Jia Yang

**Co-supervisors:** Prof.em. Anders Holmen and Research Scientist Rune Myrstad

The depletion of oil reserves has increased the interest in developing and improving processes that can replace the use of crude oil. An alternative is the Fischer Tropsch synthesis (FTS), a catalytic process where syngas ( $\text{CO} + \text{H}_2$ ) reacts to form a range of hydrocarbons, such as light olefins, gasoline, diesel and waxes. The lower olefins ( $\text{C}_2\text{-C}_4$ ) and their derivatives are important building blocks in the chemical industry, used to produce many high performance materials and chemical products, i.e. plastic and engineering resins, lubricants, coatings and paints. To increase the renewability of the process, the syngas feedstock should derive from biomass. However, syngas from biomass is lean in hydrogen, and can be rich in  $\text{CO}_2$  if extensively removed. This makes iron an attractive catalyst, as it can manage a relatively wide range of syngas feed ratios ( $\text{H}_2/\text{CO} = 0.5\text{-}2.5$ ), due to the water-gas-shift activity, additionally it can work at higher temperatures with low methane production. However, iron catalyst are prone to deactivation by sintering, catalyst attrition, phase-transformations and carbon deposition.

This project aims at synthesizing novel iron-based catalysts, which involves pyrolysis of iron-containing polymers, to form iron nanoparticles supported on porous carbon. The synthesis conditions will be optimized in order to achieve a highly active and stable catalyst for the FTS. Iron species, particle size and distribution, and morphology will be investigated by the use of Powder XRD, S(T)EM, TEM and XAS, and BET and Raman for porosity and carbon characteristics respectively. The effect of promotion by potassium and activation method on selectivity, activity and stability will be tested in the high-pressure FT rig, while operando studies with XRD and XAS will give valuable information on their effect on the iron species in the catalyst. Mechanistic insight will be obtained by SSITKA.

### **Financial support:**

The project is funded by Faculty of Natural Sciences, Norwegian University of Science and Technology (NTNU)

## Nanoscale Investigation of Co(0001), Co(10-12), and Co(11-20) Single Crystals as Catalyst Model Systems: Insights from Experiment and Theory

**Researchers:** Dr. Mehdi Mahmoodinia, Dr. Marie Døvre Strømsheim, Dr. Mari Helene Farstad

**Supervisors:** Professor Hilde Johnsen Venvik and Adjunct Associate Professor Ingeborg-Helene Svenum

Single crystals provide model systems that can further the understanding of phenomena occurring at the surface of a catalyst e.g. adsorption/desorption, reaction, surface segregation, reconstruction, promotion and poisoning. Understanding the dynamic surface of a cobalt (Co)-based Fischer Tropsch (FT) catalyst motivated the work with the Co single crystals.

In the Co-based Fischer-Tropsch synthesis (FTS) reaction, the carbon and oxygen atoms of the CO precursor molecule react with surface hydrogen atoms to form  $C_xH_y$  and  $H_2O$ . The idea is to increase the selectivity of this reaction in order to produce long chain aliphatic hydrocarbons at relatively low temperature, around or below 500 K. The active phase of industrially applied cobalt catalysts consists of metallic nanoparticles, which expose a heterogeneous surface with a large variety of active sites (corners, edges, steps, kinks, reconstruction). Therefore, a fundamental understanding of the adsorbates on different Co surfaces and the elementary reaction steps involved is an essential tool for catalyst design and optimization in the FT synthesis. Three different single crystal surfaces of cobalt were used to address this question: Co(0001), Co(10-12) and Co(11-20). A combination of density functional theory (DFT) study, temperature programmed desorption (TPD) and low electron energy diffraction experiments in collaboration with SynCat@DIFFER research lab in Eindhoven, the Netherlands, have been used to gain insight into the structure of cobalt surfaces upon adsorption of  $H_2$  and CO and to study the adsorption strength of hydrogen atoms or CO as a function of surface structure and surface coverage.

One of the important elementary reaction steps in the FTS process is the dissociative adsorption of  $H_2$  on the Co surface, to enable the hydrogenation steps on the surface. One question is how the surface structure of cobalt catalysts affects the  $H_2$  dissociation and the adsorption strength of atomic hydrogen. Our results demonstrate that the influence of surface structure on the adsorption and dissociation of hydrogen is surprisingly large. The TPD data showed lower desorption temperatures for hydrogen atoms on the more open surfaces. This is in agreement with the results from DFT calculations for both low and high coverage, finding that hydrogen adsorbs weaker on the corrugated (11-20) and (10-12) surfaces compared with the flat (0001) surface. The insight into the lateral interactions between adsorbed hydrogens was also investigated using DFT calculations as we sequentially increased the surface hydrogen coverages. The results were qualitatively in line with the trend in the desorption temperatures observed in the TPD spectra for the three surfaces. In the context of hydrogenation of CO over supported Co particles, our study agrees with previous work suggesting that undercoordinated Co sites are important for efficient  $H_2$  dissociation. After dissociation, diffusion of hydrogen atoms to sites with higher adsorption strength on the flat terrace is facile, making it available for hydrogenation reactions.

The surface of Co(11-20) is known from previous work in the group to reconstruct upon exposure to CO at room temperature, with scanning tunneling microscopy (STM) results showing that adsorption of CO ( $\sim 1 \cdot 10^{-9}$  mbar) at room temperature on clean Co(11-20) induces a (3x1)-reconstruction of the surface. This reconstruction involves the anisotropic transport of Co from and to the step edges. However, it is not possible to discern from the STM images if

Co is migrating in clusters, single atoms or as a carbonyl, nor the adsorption site of CO on the reconstructed Co surface or the coverage of the CO-saturated surface.

The STM results were used to select three theoretical model systems, one for the unreconstructed surface (1x1) and two with a (3x1) periodicity of either an added or missing row, to model the reconstruction. Slightly higher stability was obtained for CO on the reconstructed surfaces, with CO in coordination with the added row yielding the lowest calculated adsorption energies. The TPD measurements showed that the desorption temperature for CO adsorbed on an unreconstructed surface was only slightly lower than from a reconstructed surface together with a somewhat higher coverage on the reconstructed surface near room temperature. Transition state calculations with climbing image nudged elastic band (CI-NEB) were performed to investigate the removal of a Co atom from the topmost layer and its mobility across the surface and the results indicated that the migration under CO exposure occurs in the form of a carbonyl.

### **Publications and Conference contributions in 2018:**

Weststrate, C.J. (Kees-Jan); Mahmoodinia, M.; Farstad, M.H.; Svenum, I.-H.; Strømsheim, M.D.; Niemantsverdriet, J.W. (Hans); Venvik, H.J., Interaction of Hydrogen with Flat (0001) and Corrugated (11–20) and (10–12) Cobalt Surfaces: Insights from Experiment and Theory. *Catalysis Today*, DOI:10.1016/j.cattod.2019.04.002.

Weststrate, C.J. (Kees-Jan); Mahmoodinia, M.; Farstad, M.H.; Svenum, I.-H.; Strømsheim, M.D.; Niemantsverdriet, J.W. (Hans); Venvik, H.J., Hydrogen Adsorption on Co Surfaces: Insights from Temperature Programmed Desorption and Density Functional Theory Study. 2018 iCSI annual seminar, 2018-11-19 –2018-11-20, Selbu, Norway.

Mahmoodinia, M., Challenges in Catalysis Science and the Role of DFT Modelling; iCSI Workshop 2018 “Challenges in Catalysis Research”, 2018-11-05 –2018-11-06, Langesund, Norway.

Mahmoodinia, M.; Åstrand, P.-O.; Chen, D., Single-atom and Dimer Pt Catalysts Supported by Graphene Nanomaterials: Quantum Chemical Calculations. Cluster-Surface Interactions Workshop (CSI2018); 2018-06-18 – 2018-06-21, Trondheim, Norway.

MD Strømsheim, I-H Svenum, MH Farstad, K-J Weststrate, A Borg, HJ. Venvik, The CO-induced surface reconstruction on Co(11-20)– a combined theoretical and experimental investigation. ECOSS-34 (26th – 31st of August, Aarhus, Denmark) – oral contribution.

MD Strømsheim, I-H Svenum, MH Farstad, K-J Weststrate, A Borg, HJ. Venvik, The CO-induced surface reconstruction on Co(11-20)-a combined theoretical and experimental investigation Norwegian Catalysis Symposium - Landsmøte i kjemi (October 16th-17th 2018) - oral contribution:

MD. Strømsheim, MH Farstad, I-H Svenum, K-J Weststrate, L Gavrilovic, S K. Regli, Z Li, A Borg, Hilde J. Venvik, The effect of K on the adsorption and decomposition of ethylene on Co(11-20). Tailor2018 (June 11-14 2018, Ystad, Sweden) – oral contribution.

### **Financial support**

The research has been performed with support from the Department of Chemical Engineering, NTNU, and the Research Council of Norway under the contracts 280903, 237922 and 174893/O30. The computations were performed on resources provided by UNINETT Sigma2 - the National Infrastructure for High Performance Computing and Data Storage in Norway (account nn9152k and nn9355k) and local resources on Vilje, account no. ntnu946. Syngaschem BV provided financial support for the experimental investigations.

## Advanced characterization of Pd-based membrane model systems

**Postdoctoral fellow:** Marie D. Strømsheim

**Project organization:** Professor Hilde J. Venvik, Research Scientist Dr. Ingeborg-Helene Svenum (SINTEF), Senior Scientist Dr. Thijs Peters (SINTEF), Guest researcher Dr. Mehdi Mahmoodinia, Master student Gaute Osaland Hådem

The postdoctoral work is part of the H2MemX-project, a joint effort between NTNU and SINTEF, and in cooperation with Lund University/the MAXIV Laboratory, to advance the understanding of Pd-based membranes for hydrogen separation from gas mixtures. Further knowledge of these membranes is desirable as they may enable the production of high purity hydrogen regardless of the feedstock (biomass, natural gas). The specific focus of the postdoctoral project is the investigation of the surface chemistry and segregation phenomena of the Pd-alloy membranes/model systems (i.e. single crystals), under conditions as near as possible to application. The overall aim is to apply the insight of segregation phenomena and changes in surface chemistry and composition under these conditions towards tuning membrane performance and stability. The Pd/Pd-alloy membranes are manufactured by SINTEF through a two-step sputtering method of the desired Pd and alloy material on to a Si substrate. This method allows for easy separation of the membrane from the substrate and application to a wide range of support configurations, as well as control of the thickness and composition of the resulting membranes.

The separation of hydrogen from the other components of the gas mixture occurs through H<sub>2</sub> dissociating on the Pd surface of the feed (high pressure) side, diffusing through the bulk metal matrix, and recombining on the permeate (low pressure) side of the membrane. Hydrogen absorption in pure Pd can lead to a phase transition ( $\alpha \rightarrow \beta$ ), which is detrimental to the mechanical stability of the membranes under the relevant industrial conditions for hydrogen separation. Hence alloying with Ag, Au or Cu is, among other reasons, carried out as a counter measure, without a large resulting change in the permeability. However, the introduction of a secondary metal requires insight into segregation phenomena as the surface composition changes upon exposure to different gaseous environments as well as various conditions (T,P). The segregation behavior and surface chemistry under various chemical environments and conditions (T,P) of Pd-alloy membranes and model surfaces (single crystals) will be elucidated with ambient photoelectron spectroscopy (APPES). The investigation of the membrane surfaces under hydrogen permeation will be realized through the design of a reaction cell in collaboration with the MAX IV Laboratory in Lund, Sweden. This reaction cell will be installed in the synchrotron facility to allow in-situ characterization with APPES with pressures on the analyzed side in the mbar-range.

### Presentations in 2018:

Svenum, I.-H.; Vicinanza, N.; Herron, J.A.; Mavrikakis, M.; Venvik, H.J.; Effects of Surface Phenomena on the Performance of Pd-Ag Membranes, Tailored surfaces in operando conditions (Tailor2018), 2018-06-11 – 2018-06-14, Ystad, Sweden – oral contribution.

Hådem, G.O.; Mahmoodinia, M.; Svenum, I.-H.; Strømsheim, M.D.; Venvik, H. J., Nanoscale Investigation of Pd<sub>3</sub>Au(100) Single Crystal as a Model System for Hydrogen Separation. The 2018 eSSSENCE meeting on Multiscale modelling of materials and molecules; 2018-06-11 – 2018-06-13, Uppsala, Sweden.

Hådem, G.O.; Mahmoodinia, M.; Svenum, I.-H.; Strømsheim, M.D.; Venvik, H. J., Nanoscale Investigations of Pd<sub>3</sub>Au(100) Single Crystal as a Catalyst Model System. Time, Work and Function: Time-Resolved Synchrotron and Neutron Techniques for Studies of Soft, Biological and Hard Matter (TWF2018); 2018-06-13 – 2018-06-15, Oslo, Norway.

**Financial support:**

The research is performed with financial from the Research Council of Norway (Contract no. 280903) and the Department of Chemical Engineering, NTNU.

## Low Cost Drill Bit for Geothermal Applications

**Researcher:** Xiaoyang Guo

**Supervisor:** Associate Professor: Jia Yang

**Co-supervisor:** Professor: De Chen

The underlying idea of the project is to reduce the cost of polycrystalline diamond compact, PDC, (fixed cutter) drill bits, currently used extensively in the oil and gas industry, to a cost - level that makes them competitive in geothermal applications. The current preferred drill bit types in geothermal applications are roller cone drill bits. These drill bits have a low cost and can drill just about any rock type. The major drawbacks associated with roller cone bits are low drilling speeds (inefficient), low durability (due to moving parts) and low temperature tolerance (due to use of seals).

Roller cone drill bits are still used in oil & gas wells but have more or less been replaced by PDC drill bits in all hole sizes smaller than 17 ½” due to superior rate of penetration, ROP, (drilling speed) and durability (meters drilled). In addition, a PDC drill bit is far less sensitive to downhole temperatures; a critical feature in deep geothermal applications. The major drawback with PDC drill bits is the cost. The cost drivers for PDC drill bits are the PDC cutters and the body material. The proposed project will focus on reducing the cost of the body material and new, lower cost manufacturing methods

Tungsten carbide (WC) is the base material in commercial drill bits today. Tungsten is heavy, very expensive, with limited resources on earth and on the list of critical raw materials. In the previous project in our group, attempts were made to apply SiC, in place of WC in order to significantly reduce cost (and weight) of final drill bits while keeping high mechanical strength. Serious challenges were faced in form of poor wetting of the SiC ceramic body with the infiltration alloy, resulting in poor penetration of the infiltrate into the SiC body. Further development is hence required to focusing on the development of extreme hard-material by coating technology through wet chemistry and gaseous treatment.

The basic idea is to overcome the wetting issues faced with SiC in the previous project by synthesis of WC coating on SiC (WC@SiC, core-shell structures). The kinetic and thermodynamics of the carburization process is very intricate, and the challenge is to grow/synthesize single phase WC with nanometer size, which has good wettability with typical binder materials (CuNiMn based alloys). The uniformity of the WC coating and integrity of the nanocomposite is also crucial for the infiltration process and the strength of the final drill bit produced. Evaluation of the use of this powder for 3D printing will also be performed.

### **Financial support:**

The project is funded by Lyng Drilling, Schlumberger, Norwegian Research Council and the Department of Chemical Engineering, NTNU.

## **Low-temperature post-combustion CO<sub>2</sub> capture using solid amine sorbents**

**Researcher:** Dr. Qingjun Chen

**Supervisor:** Prof. De Chen

The development of novel materials and new technologies for CO<sub>2</sub> capture and storage has received great attentions due to the global warming issues. The CO<sub>2</sub> capture by solid amine sorbents could diminish the environmental impact of CO<sub>2</sub> capture in liquid amine absorption and at the same time have a lower energy penalty, thus it may be a promising technology for CO<sub>2</sub> capture in the future. This work emphasized on the synthesis of PEI-impregnated mesoporous carbon spheres (MCS) with high CO<sub>2</sub> capture capacity and fast kinetics, which can be used in fluidized bed reactor or moving bed reactor for low-concentration CO<sub>2</sub> capture from natural gas power plant.

The MCS were prepared by a hard-template assisted reverse emulsion method from carbon precursors and silica nanoparticles template. The pore structures of the MCS were tuned by changing the type and amount of silica nanoparticles. The diameters of the MCS were adjusted by altering the concentration of surfactant (span 80) and polymerization condition. PEI-impregnated MCS were prepared by a wet impregnation method. The results showed that perfect spherical morphology of the MCS was achieved with very smooth and clean surface. The diameters of the MCS were very homogeneous and in the region of 0.3-0.4 μm. The N<sub>2</sub> adsorption results of MCS indicate the co-existence of micropores and mesopores/macropores. The micropore volumes of MCS are similar and mesopore/ macroporous volume increased with content of silica nanoparticles. The total volume and surface area of MCS were up to 2.68 cm<sup>3</sup>/g and 1097 m<sup>2</sup>/g, respectively. The developed pore structure of MCS allows a high amount of PEI loading (>60 wt%) with good dispersion.

The optimal PEI loading of the sorbent depends on the pore structure of MCS. The PEI-impregnated MCS with medium pore volume (1.64 cm<sup>3</sup>/g) and PEI loading (63 wt%) exhibited the highest CO<sub>2</sub> capacity of 3.22 mmol/g, which outperforms other solid amine sorbents reported at similar condition. The adsorption temperature also significantly affects the CO<sub>2</sub> capacity. There is a balance between the CO<sub>2</sub> adsorption/desorption and diffusion in the PEI film in the sorbent. 75 °C is the optimal temperature for the CO<sub>2</sub> adsorption over PEI/MCS. The PEI impregnated MCS also exhibited fast sorption/desorption kinetics and excellent regeneration performance (>99%). A continuous fluidized bed reactor will be built and the CO<sub>2</sub> capture in the cycling fluidized bed reactor will be verified.

### **Publications and Presentations in 2018:**

1. Qingjun Chen, Ingeborg-Helene Svenum, Yanying Qi, Ljubisa Gavrilovic, De Chen, Anders Holmen, Edd A. Blekkan, Effect of trace potassium on hydrogen adsorption and dissociation on hcp cobalt: A density functional theory study, *Surface Science*, 2019, 681 24-31.
2. Qingjun Chen, Siyu Wang, Kumar R. Kent, De Chen, Development of polyethylenimine (PEI)-impregnated mesoporous carbon spheres for low-concentration CO<sub>2</sub> capture from natural gas power plant, CLIMIT PhD and Post Doc Seminar, Oslo, Norway, 2019, Poster presentation.

### **Financial Support:**

This project is financed by the CLIMIT program (LCP3T) in the Norwegian Research Council.

## **Fundamental study of CuCl<sub>2</sub>/γ-alumina catalyzed ethylene oxychlorination and methanol oxidation**

**Postdoctoral fellow:** Yanying Qi

**Supervisors:** Prof. De Chen

Ethylene oxychlorination is an important step in the industrial production of vinyl chloride monomer (VCM), which is needed for polyvinyl chloride (PVC) production. CuCl<sub>2</sub>/γ-Al<sub>2</sub>O<sub>3</sub> based catalysts are effective to catalyze ethylene, HCl and oxygen to produce 1,2-dichloroethane (EDC) in this process. In this project, we performed DFT calculations to investigate the nature of active phase and to understand the promoter effect.

We built a new model to present CuCl<sub>2</sub> supported on γ-Al<sub>2</sub>O<sub>3</sub>. The new model involves the contribution of support, which is more close to the real catalyst compared with the previous model (i.e., CuCl<sub>2</sub> surface). Based on the new model, the adsorption behaviors of ethylene at different loadings were investigated. Distinct adsorption modes at high loadings and low loadings were observed and the underlying reason was discovered by the analysis of the electron properties, such as Bader charge analysis.

Besides, we built a model with CuCl<sub>2</sub> molecules and KCl molecules on γ-Al<sub>2</sub>O<sub>3</sub> to study the promoter effect of potassium. The KCl binds with CuCl<sub>2</sub> molecules, indicating a K<sub>x</sub>Cu<sub>y</sub>Cl<sub>z</sub> salt is formed on the alumina surface. The effect of KCl on ethylene adsorption depends on the Cl/Cu ratio. It weakens ethylene adsorption heat and thus increases the reduction barrier at a high Cl/Cu ratio, while it has a negligible effect on the adsorption energy of ethylene at relatively low Cl/Cu ratios. Moreover, KCl increases the adsorption strength of oxygen and decreases the barrier of oxygen dissociation compared to the neat Cu<sup>+</sup> catalysts.

We performed micro-kinetic modeling for methanol oxidation reaction. It is found that both O-assisted and OH-assisted reaction pathway could decrease the reaction barrier and thus improve the activity compared to the direct methanol decomposition. O-assisted methanol dissociation is suggested to be the most favorable reaction pathway by analysis of the free energy profiles and oxygen dissociation is the rate determining step in this mechanism. We will search other alternative reaction mechanism in order to reduce the barrier of the rate determining step (i.e., oxygen dissociation).

### **Financial support:**

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



## Conversion of lignocellulosic waste into biofuels and bioplastics

**Postdoctoral Fellow:** Zhenping Cai

**Supervisor:** Prof. De Chen

The dwindling of petroleum resources and global environment problem have forced a rethink on the continued use of fossil fuels and focus on renewable resources valorization such as lignocellulosic biomass, which is expected to be the most promising feedstock owing that it does not increase the level of CO<sub>2</sub> in the atmosphere and wide abundance. To date, bench-scale depolymerization technologies such as pyrolysis, gasification, liquefaction, and hydrogenolysis have been shown to convert biomass into bio-oil and value-added chemicals.

Lactic acid, an industrially important chemical widely used in food, pharmaceutical, and bioplastics, can be catalytically produced from several feedstocks, such as biomass, cellulose and sugars. Both heterogeneous and homogeneous catalysts have been employed to catalyze the reactions. For example, metal ions have been used to produce directly from lignocellulosic biomass under subcritical water. And several types of heterogeneous catalysts such as zeolites, sulfonated carbon, sulfated zirconia, tungstated alumina, and heteropolyacids was also investigated. However, the low yield and selectivity with harsh reaction conditions limit the commercialization of this chemical route. As a result, development of novel efficient catalysts for selective conversion biomass and cellulose into lactic acid should be paid much attention. In this project, we focus on the direct production of lactic acid as the feedstock of bioplastics. Global consumption of bioplastics for packaging is projected to grow to just over 2 million tons by 2020, with a market value of almost \$5 billion. In particular, polylactic acid (PLA) is a transparent plastic and biodegradable polymer which is used in the plastic processing industry for the production of films, fibers, plastic containers, cups and bottles. Moreover, the use of low cost biomass as feedstock for PLA generation makes our process economically viable. Here, we proposed a series of novel single-site tungsten oxide supported catalysts for conversion of cellulose into lactic acid directly.

### **Financial support:**

The work is supported by Norwegian Research Council through the the project of CONVERSION OF LIGNOCELLULOSIC WASTES INTO BIOFUELS AND BIOPLASTICS in the INNO INDIGO program

## Catalysts for alkaline ethanol fuel cell

**Postdoctoral fellow:** Jørgen Svendby

**Supervisor:** Prof. De Chen

**Co-supervisor:** Assoc. Prof. Jia Yang

Fuel cells are regarded as part of the solution for the transition from a world based on non-renewable energy sources to one based on renewable energy sources. Efficient, easy to scale up, high energy density, quiet, and negligible emissions make the fuel cell an ideal candidate from everything to power neighborhoods and buildings to the use in cars to laptops and other electrical devices.

Hydrogen has shown to be the best fuel, with a high energy conversion yield and almost no over-potential for its electrochemical reaction. Unfortunately, hydrogen is difficult to store and distribute because of its gaseous state. This is particularly challenging if used in non-stationary applications where low weight and volume are important. Therefore, liquid fuels like ethanol have received some attention.

Ethanol is easy to store and handle, in addition to be relatively safe. It can easily be produced in large volumes from several sources at a low cost. The problems with ethanol are a significantly over-potential during its oxidation and the low overall efficiency of the cell. In addition, high costs because of expensive materials is a general problem for fuel cells, so also for ethanol fuel cells. By using an alkaline based cell makes it possible to use cheaper materials because of a less hostile environment, in addition to better performance compared to an acidic based one. This makes it possible to develop and use cheaper catalysts and still maintain good cell performance. In this project the goal is to develop catalysts with high performance and low costs, where the target is to develop a catalyst performing better than the commercial Pt-catalyst.

The project started investigating non-PGM catalysts, but it was soon evident that PGM-metals had to be included. Several synthesis methods have been tested, mostly with an undesirable performance. Pd- and PdNi-catalysts have been developed that performs better than commercial Pt. Further testing will be conducted, in addition of testing other Pd-based catalysts.

### **Financial support:**

This project is part of the NanoElMem which is financed by M-ERA.NET, an EU funded network financed under the project number 4228.

## Moving Bed Carbonate Looping (MBCL), Phase I and II

**Participants:** Prof De Chen, NTNU, Kumar R Rout, SINTEF, Torleif Madsen, FTG, Asbjørn Strand, FTG, Li He, NTNU, Ainara Moral Larrasoana, NTNU, Yuanwei Zhang, NTNU

In CLIMIT project MBCL phase I, the concept of heat integration to calciner is done by catalytic combustion, where modified dolomite sorbent is considered and process efficiency is calculated using ASPEN. It is found that the energy efficiency of NGCC power plant with PCCC is 55.9% points, whereas the NGCC plant without CO<sub>2</sub> capture is 57.6% point, as reported by MBCL phase I Q1-Q2 report. The energy penalty of CO<sub>2</sub> capture is about 1.7%. This is the best efficiency and lowest of energy penalty that are ever published for NGCC power plant integrated with PCCC. It is noted that the proper heat integration is essential to increase the energy efficiency of the power plant. More importantly, beyond power generation the developed methodology possesses highest potential to increase the energy efficiency of MEA plant and post-combustion CO<sub>2</sub> capture for H<sub>2</sub> production from natural or bio-gas.

An innovative moving bed reactor (MBR) is proposed in the MBCL phase I and is reported in our filed MBCL patent II. In the MBR, one or more mass transfer regions are arranged such that, the solid reactant is retained within the one or more mass transfer regions as the solid reactant flows through the mass transfer system and the mass transfer between the gas and the solid reactant occurs in the one or more mass transfer regions. Extensive research has been done before in order to produce a cost efficient chemically and mechanically stable solid sorbent including our effort to our previous patent (NTNU). For the 430 MW power plant we need 80 ton of solid inventory to capture 85% of CO<sub>2</sub>. The reported solid sorbent cost varies from 2800-4600 USD/ton, which is not feasible for the CCS scenario at an industrial scale. Therefore, effort is made in the MBCL phase I to produce chemically stable doped dolomite solid sorbent by utilizing our previous patent (NTNU) and our doped dolomite cost around 750 USD/ton (MBCL phase I Q2-Q3 report).

Cost evaluation of MBCL plant, i.e., CAPEX and OPEX is done and compared with conventional MEA plant. The MBCL system can decrease annual cost by 32.2% and net cost of CO<sub>2</sub> avoided is reduced by 42.4% in comparison to MEA system (MBCL Phase I Q2-Q3 report). A sensitivity analysis is done by varying the important cost parameters, i.e., increasing contingency, sorbent make-up, operational cost by 100% and increasing the MBCL plant energy penalty two fold, it is found that the MBCL still would be a preferred technology in comparison to MEA technology.

The doped dolomite sorbent is tested for ca 200 carbonation and calcination cycles using dry condition and the sorbent possess excellent chemical stability (MBCL Phase I Q2-Q3 report). However, in the real flue gas from the NGCC power plant contains water vapour; thus it is essential to study the doped dolomite powders in the wet condition. Efforts has been made to study the doped dolomite capture behaviour in the wet condition and the sorbent powder possess excellent capture capacity (above 0.1 gCO<sub>2</sub>/g-sorbent) and stability for ca 50 carbonation and calcination cycle (MBCL Phase I Q2-Q3 report), which is best reported data yet. In the real industrial application, we need solid sorbent pellet instead of powder, which should have not only good chemical stability but also excellent mechanical stability. We have developed doped dolomite pellets using high shear granulator by doping binders to increase mechanical stability (MBCL Phase I Q2-Q3 report). The mechanically stability from our doped pellets has excellent mechanical stability from our initial investigation and possess good sphericity, which is

important for good flow of solids in the reactors. A new, one step procedure to combine materials doping and palletisation is developed to simplify the process, thus decrease pellet production cost.

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

In parallel to the technological process, the project will start a process for commercialization. There will be identified and selected potential partners, increasing resources for the next phases.

#### **Patents and publications in 2018:**

Chen D., Rout, K. R., Strand, A. Gas capture system, UK patent, GB2560347

Chen D., Rout, K. R., Strand, A. method and system for gas capture comprising by circulating sorbent, International Patent, WO/2018/162675

Strand A, Rout, K. R., Chen D. Moving Bed Reactor for gas-solids reactions, UK patent Filled, 2017, GB1721034.5

Strand A, Rout, K. R., Chen D. Moving Bed Reactor for gas-solids reactions, International patent Filled, 2018, PCT/EP2018/085300

Strand A, Rout, K. R., Chen D. Moving Bed Reactor for gas-solids reactions, UK patent Filled, 2018, GB1817072

Chen, D., He, L., Rout, K. R., Blekkan, E. A. Pellets of sorbent suitable for carbon dioxide capture, UK patent filed, 2018, GB1810620.3

Chen, D., Rout, K. R., Strand, A. Gas turbine design for H<sub>2</sub> fired power plant, UK patent filed, 2019, GB1902131.0

He, L., Rout, K. R., Strand, A, Blekkan, E., Chen, D., The 5th International Conference on Chemical Looping, 2018, USA

## 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:** Equinor TCMD

### Refinery operations / Octane processes

**Staff:** Research scientist Hilde Bjørkan, Senior engineer Camilla Otterlei and Senior scientist Torbjørn Gjervan

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

**Client:** Equinor ASA

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

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

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

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

The main objectives of 4REFINERY are:

- To develop new biofuels production technology while at the same time increase understanding and control of the entire value chain

- To scale up materials and testing procedures to define scenarios for the best further implementation in existing refineries
- To develop solutions to answer key societal & environmental challenges

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

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

### **Biofuels from waste to road transport (Waste2Road, 2018 – 2022)**

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

**Project category:** Horizon 2020, "Development of next generation biofuel and alternative renewable fuel technologies for road transport"; SINTEF is project coordinator (Duncan Akporiaye), project manager Jana Chladek

Waste2Road will develop a new generation cost-effective biofuels from low cost and abundant biogenic residues and waste fractions. This will be achieved through optimization of European waste recycling logistics and development of efficient conversion technologies, giving carbon yields > 45% with greenhouse gas (GHG) savings > 80%. The consortium will deploy risk-mitigation pathways to realise industrial implementation, with primary processing at European waste recycling sites and co-processing within European refineries. SINTEF will study catalytic hydrotreating and co-hydrotreating of pyrolysis oils and hydrothermal liquefaction oils from different resources at laboratory and semi-pilot scale with full pellet catalysts. The work involves optimization of catalyst as well as process parameters.

The main objectives of Waste2Road are:

- To develop a representative and cost-effective waste supply and management system to reduce and optimize the supply costs while diversifying the biomass feedstock basis.
- To develop new biofuels production technology while increasing understanding and control of the whole value chain.

- To scale up materials and testing procedures to define scenarios for the best exploitation through implementation of process schemes in existing refineries
- To develop solutions to answer key societal & environmental challenges.

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

**Staff:** Senior Scientist Rune Lødeng

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

Distribution of liquefied natural gas (LNG) is developing in Norway as well as globally, and represents an option for efficient and more environmental friendly marine propulsion. With LNG as fuel it is critical that methane emissions (slip) are controlled to very low levels since methane is a greenhouse gas with more than 20 times the global warming potential than CO<sub>2</sub>. The proposed project targets new knowledge and innovation for emissions abatement, more specifically nitrogen oxides (NO<sub>x</sub>) and methane (CH<sub>4</sub>) in the marine sector. It is a collaboration project between NTNU and SINTEF. NTNU is focused on selective catalytic reduction and SINTEF is focusing on methane abatement for natural gas engines in the marine sector. Success criteria are to obtain > 90% methane conversion below 500 oC in excess of oxygen, presence of H<sub>2</sub>O and CO<sub>2</sub>, and possibly also potential poisons like NO<sub>x</sub>, NH<sub>3</sub>, SO<sub>x</sub> and S (from fuel, lubricant or added as odorant). Highly active and stable catalysts based on transition metal oxides are under development. Noble metals are included in the study as reference materials.

**Publications:**

Jia Yang, Rune Lødeng, Hilde Venvik, Catalytic methane oxidation for emission control, Oral presentation (Jia) at 9th ICED, Newcastle, Australia (10 – 13. July, 2016)

Jia Yang, Rune Lødeng, Hilde Venvik, Co and Ni spinel catalysts for low temperature methane total oxidation, Poster P3.279 Europacat 2017, 29 – 31 August, Florence Italy

Jia Yang, Ragnhild Lund Johansen, Rune Lødeng, Hilde J. Venvik, Co and Ni spinel catalysts for low temperature methane total oxidation, Poster iCSI/NKS meeting, Hurdalssjøen 6. – 7. November 2017

**Client:**

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

## **Benchmarking low temperature shift catalysts**

**Staff:** Senior Scientist Bjørn Christian Enger, Research Scientist Rune Myrstad

The goal of this project is to support the client's efforts in selecting catalysts for gas conditioning. This involves testing of commercial catalysts using the client's conditions and analysis of gaseous and liquid products.

**Client:** Borealis

## **Pulp and Paper Industry Wastes to Fuel (Pulp&Fuel 2018-2022)**

**Staff (WP2):** Fuel synthesis and product management): Senior Scientist Bjørn Christian Enger (work-package leader), Research Scientist Rune Myrstad, Research Scientist Håkon Bergem, Research Scientist Julian Richard Tolchard, Research Scientist Kumar R. Rout

**Project category:** EU Horizon 2020, "Development of next generation biofuels and alternative renewable fuel technologies for road transport"; CEA Liten is project coordinator.

The transport sector is dominated by the use of fossil fuels, and alternative fuels represent currently only 5% of fuel consumption in EU. The EU objective for the share of renewable energy in the transport sector is 10% in 2020. To achieve this goal, new advanced biofuels are needed and must be produced from alternative feedstocks.

The Pulp&Fuel concept is to develop a simple and robust fuel synthesis process taking advantage of the synergy between super critical water gasification (wet gasification) and fixed bed gasification (dry gasification).

For the Pulp&Fuel project, we have chosen to study the integration of the full process on a pulp mill. The developed process will take advantage of low to negative value wet and dry resources on a paper mill to add value to the overall process. The yield of biofuels will be significantly increased to 28 % compared to a classic approach that would only yield 18 %. The Pulp&Fuel final objective is to produce biofuels below 1 €/L without having a negative impact on the existing operations of the pulp mill. To achieve these goals a team of 10 partners, leaders in their field, from 4 EU-member states, will join efforts. The Pulp&Fuel project addresses the topic "liquid diesel- and gasoline-like biofuels from biogenic residues and wastes through either chemical, biochemical and thermochemical pathways, or a combination of them" of the LCSC3-RES-21-2018 call.

**Client:** EU



## **Gasification and FT-synthesis of lignocellulosic feedstocks (GAFT)**

**Staff:** Research Scientist Rune Myrstad and Senior Scientist Bjørn Christian Enger: SINTEF

**Project category:** KPN-project in ENERGIX. Project responsible is SINTEF Energy Research

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

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

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

## **Moving Bed Carbonate Looping (MBCL)**

**Key team:**

**Fjell Technology Group (FTG, the owner of the project):** Torleif Madsen (Administrative Management), Dr. Asbjørn Strand (Project Management and R&D Specialist), Jonny Vassdal (Mechanical Design Specialist), Leif Gunnar Madsen (CEO, Commercialisation)

**NTNU:** Prof. De Chen, Prof. Edd A. Blekkan, Dr. Li He, Post doc Ainara Moral Larrasoana, Post doc Yuanwei Zhang, Assoc. Prof. Kumar R Rout

**SINTEF:** Dr. Kumar R Rout

The moving bed carbonate looping concept (MBCL) has been developed by NTNU/SINTEF/FTG since 2017. In CLIMIT demo project MBCL phase I, the concept of heat integration to calciner is done by catalytic combustion, where modified dolomite sorbent is considered and process efficiency is calculated using ASPEN. It is found that the energy efficiency of NGCC power plant with PCCC is 55.9% points, whereas the NGCC plant without CO<sub>2</sub> capture is 57.6% point, as reported by MBCL phase I Q1-Q2 report. An innovative moving bed cold flow reactor (MBR) is developed in the MBCL phase II. In the MBR, one or more mass transfer regions are arranged such that, the solid reactant is retained within the one or more mass transfer regions as the solid reactant flows through the mass transfer system and the mass transfer between the gas and the solid reactant occurs in the one or more mass transfer regions.

The doped dolomite sorbent is tested for ca 200 carbonation and calcination cycles using dry condition and the sorbent possess excellent chemical stability (MBCL Phase I Q2-Q3 report). However, in the real flue gas from the NGCC power plant contains water vapour; thus it is essential to study the doped dolomite powders in the wet condition. Efforts has been made to study the doped dolomite capture

behaviour in the wet condition and the sorbent powder possess excellent capture capacity (above 0.1 gCO<sub>2</sub>/g-sorbent) and stability for ca 50 carbonation and calcination cycle, which is best reported data yet. A new, one step procedure to combine materials doping and palletisation is developed to simplify the process, thus decrease pellet production cost.

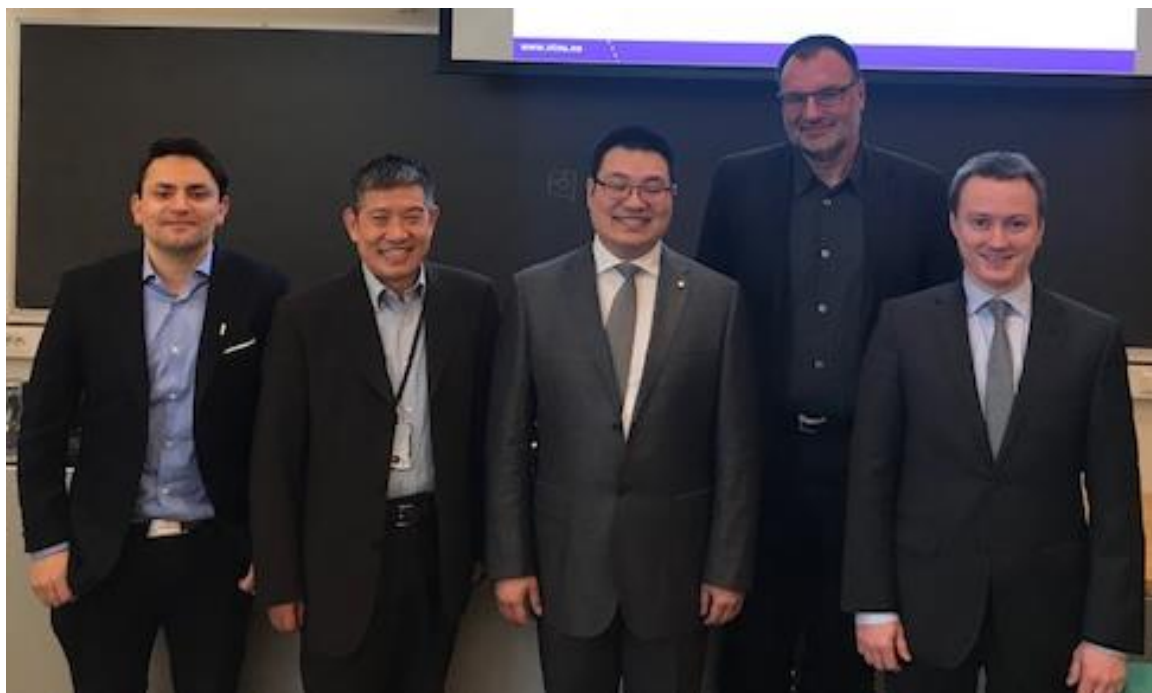
Apart from this a kinetic study is done and a kinetic model based on ion migration hypothesis is developed, which is implemented MBCL hot (numeric) reactor model. Cold flow MBCL reactor consists of multi-channel carbonator, calciner MBR and riser. The cold flow integrated reactor is an important step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

**Financial Support:**

The MBCL project is financially supported by GASSNOVA

## Philosophiae Doctor (PhD) theses in 2018

Yahao Li: *Sustainable electrocatalysts for oxygen reduction reaction. M-N-P (M:transition metals) doped mesoporous carbon from biomass.* Doctorial theses at NTNU, 2018:72.



Disputas Yahao Li: 8/3 2018. From left: Dr. Alejandro Oyarce Barnett, Prof. De Chen, Yahao Li, Prof. Martin Muhler and Prof. Johannes Jäschke

Ljubisa Gavrilovic: *Fischer-Tropsch synthesis – Influence of aerosol – deposited potassium salts on activity and selectivity of Co based catalysts.* Doctorial theses at NTNU, 2018:104



Disputas Ljubiša Gavrilović , 18/4 2018. From left: Prof. Anders Holmen, Dr. Dag Schanke, Prof. Johannes Hendrik Bitter, The Netherlands, Ljubisa Gavrilovic, Prof Edd A. Blekkan, Prof. Jana Popsteinova Jacobsen (administrator), Prof. Hilde J. Venvik.

Erik Østbye Pedersen: *Mn promotion effects in Co based Fischer-Tropsch production of light olefins*. Doctorial theses at NTNU, 2018:180



**Disputas Erik Østbye Pedersen, 18/6 2018. From left: Dr. Ole Swang, Prof. Andrei Khodakov, France, Dr. Ingeborg-Helene Svenum, Eirik Østbye Pedersen, Prof. Magne Hillestad, Prof. Edd A. Blekkan.**

## Master (Diploma) Students in 2018

Najma Ali Abdullahi: *Catalytic combustion of natural gas*

Kamilla Arnesen: *Oxidation of Methanol to formaldehyde over Ag catalysts*

Dani Espevik: *Artificial photosynthesis Visible-light photocatalysts for water splitting*

Helene M. E. Granlund: *Catalytic methane abatement for natural gas engines*

Marit Harneshaug: *Biopolymers assist preparation of Fe-based Fischer-Tropsch catalysts*

John Helms: *Initial stages of metal dusting corrosion*

Kin Hui: *New catalysts for low-temperature selective catalytic reduction (SCR)*

Signe Marit Hyrve: *Tuning of perovskite composition for NO oxidation*

Gaute O. Hådem: *Nanoscale investigations and modifications of catalysts & catalytic model systems*

Henrik Jenssen: *Efficient catalysts for achieving NO/NO<sub>2</sub> equilibrium*

Ane Sofie Lilleng: *Synthesis of solid sorbents and kinetic study for CO<sub>2</sub> capture*

Maria Oslvik: *Synthesis of solid sorbents and kinetic study for CO<sub>2</sub> capture*

Siri Stavnes: *Sorbents for sulfur removal from biomass-derived syngas*

Jonas Save: *The effect of alkali on cobalt-based Fischer-Tropsch catalysts*

Erling Olav Sollund: *Kinetic study and reactor modeling of ethylene oxychlorination*

Eline Nesdal Sundli: *Catalytic conversion of biomass derived oxygenates to fuel and chemicals*

My Nhung Thi Tran: *In situ characterization of industrial catalysts*

Amalie Tysseland: *Carbon formation and catalysis in the conversion of methylchloride and silicon into dimethyldichlorosilane*

Beate M. Østrådt: *Efficient catalysts for achieving NO/NO<sub>2</sub> equilibrium*

Jane Eiane Aarsland: *In situ characterization of industrial catalysts*



Master students at NTNU 2017-2018 (from left to right) first row standing: Kin Hui, Erling Olav Sollund, Eline Nesdal Sundli, Kamilla Arnesen, Marit Harneshaug, Helene Marie Eng Granlund, Jane Eiane Aarsland, Siri Stavnes, Gaute Osaland Hådem. Second row sitting: Amalie Tysseland, Henrik Jenssen, My Nhung Thi Tran, Beate Meisland Østrådt, Ane Sofie Lilleng, Maria Oslvik, Najma Ali Abdullahi. Photo: Estelle Vanhaecke,

## **Exchange Master Students in 2018**

Iker Hurtado Lopez: *Biopolymers assisted preparation of iron based Fischer-Tropsch catalysts*

Alizée Bataille: *(Final report delivered in France)*

Christian Mayer: *Catalytic methane abatement for natural gas engines*

## Group meetings with seminars Catalysis Group, Spring 2018

Location: Room K5-428-429

Schedule	Time	Presenter	Topic
January 26	14:00	Xiang Feng	<i>Highly Efficient Au Catalysts for Direct Propene Epoxidation with H<sub>2</sub> and O<sub>2</sub>: Structure and Performance Manipulations".</i>
February 16	14:00	Li He	<i>Process and Material Development for Moving Bed Carbonate-Looping Technology (MBCL)</i>
March 2	14:00	Ata ul Rauf Salman	<i>Catalytic oxidation of NO to NO<sub>2</sub> for nitric acid production</i>
March 8	All day	Yahao Li	<i>PhD defense</i>
March 16	14:00	Stine Lervold	<i>Ponte Vecchio - Bridging Laboratory Chemical Kinetics to Industrial Scale Reactors</i>
April 13	14:00	Jianyu Ma	<i>Chemical Looping Desulphurization under high temperature.</i>
April 17	10:15	Prof. Harry Bitter, from Wageningen, The Netherlands	<i>Non-noble metal catalysts in biobased conversions.</i>
April 18	All day	Ljubisa Gavrilovic	<i>PhD defense</i>
April 27	14:00	Qingjun Chen	<i>Design of nitrogen modified carbon spheres for low-temperature CO<sub>2</sub> capture</i>
May 25	14:00	Mehdi Mahmoodinia	<i>Electronic Structure, Stability, and Chemical Reactivity of Transition-Metal Catalysts Supported by Graphene Nanomaterials</i>
June 8	14:00	Kumar Ranjan Rout	<i>MBCL Tech: Moving Bed Carbonate Looping Technology</i>
June 18	All day	Eirik Østbye Pedersen	<i>PhD defense</i>

### Fall 2018

<b>Schedule</b>	<b>Time</b>	<b>Presenter</b>	<b>Topic</b>
September 7	14:15	Endre Fenes	<i>Calcined Al-Mg Hydrotalcite as Support in CuCl<sub>2</sub> Based Oxychlorination Catalysts</i>
September 21	14:15	Shirley Elisabeth Liland	<i>Operando study: Oxidation of NiCo/HT Catalyst for Catalytic Combustion of Methane.</i>
October 5	14:15	Ata ul Rauf Salman	<i>Catalytic oxidation of NO to NO<sub>2</sub> for nitric acid production over supported Pt Catalyst</i>
October 19	14:15	Isaac Yeboah	<i>Versatile tandem conversion of biomass-derived light oxygenates to simultaneously high yield and purity jet-fuel range aromatics.</i>
November 2	14:15	Samuel K. Regli	<i>Advanced operando characterization of heterogeneous Catalysts</i>
November 16	14:15	Yalan Wang	<i>Model-aided catalyst prediction for H<sub>2</sub> production from steam reforming through hybrid semi empirical approach.</i>
November 30	14:15	Marie Døvre Strømsheim	<i>The CO-induced surface reconstruction on Co(11-20) - a combined theoretical and experimental investigation.</i>
December 14	14:15	De Chen	<i>Sabbatical year in China</i>
December 17			<i>Julelunsj_</i>



## Guest lecture:

Please find below and attached an invitation to a presentation by Cambi.

### **From waste to worth using disruptive technologies. Challenges and opportunities**

**Time:** Wednesday 31 Oct, 14:00-14:45

**Location:** NTNU Gløshaugen, Kjemiblokk 5, room 429

**Speaker:** Dr. Farbod Dadgar

#### **Who we are:**

Cambi provides sludge management solutions for a sustainable future. Our thermal hydrolysis process (CambiTHP®) turns sewage sludge and wet organic waste into valuable resources for smarter, greener cities. Cambi's solutions reduce greenhouse gas emissions, produce renewable energy and organic fertilizers. We serve more than 70 million people in cities from 22 countries.

#### **The session:**

Cambi is continuously seeking brilliant mind and exploring R&D cooperation opportunities. In this regard, the aim is to introduce Cambi to more students and faculty members. The presentation will focus on Cambi's research and development activities, including Cambi's remote monitoring program and advance analytics, significance of sludge rheology, formation and removal of refractory organic materials.

#### **The speaker:**

Farbod Dadgar is Chemical Process Engineer at Cambi and holds an MSc in Chemical Engineering from Tehran University and a PhD (2016) in Catalysis and chemical reaction engineering from NTNU.

The presentation is open to everyone interested, especially students and employees at the Department of Chemical Engineering (IKP). Coffee and a small snack will be provided.

## Courses given by Group Members

### TKP4110 Chemical Reaction Engineering

**Coordinator:** Professor De Chen

**Lecturers:** Professor De Chen, Assoc. Prof Jia Yang, Professor Heinz Preizig (laboratory exercises)

**Semester:** Fall

**Level:** 3th year

**Credits:** 7.5 SP

**Course Plan:** Lectures (4 h/week), exercises (6 h/week), self-study (2 h/week)

**Objectives:**

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

**Prerequisites:**

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

**Contents:**

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

**Teaching form:**

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

**Course material:**

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

**Exam:** Written + exercises

## **TKP4150 Petrochemistry and oil refining**

**Responsible:** Professor Edd A. Blekkan

**Lecturers:** Prof. Edd A. Blekkan, Adjunct Prof. Kjell Moljord (Equinor), Prof. Hilde J. 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.

### **Objectives:**

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

### **Prerequisites:**

Basic chemistry and mathematics and course TKP4155 Reaction Kinetics and Catalysis or similar knowledge.

### **Contents:**

Feedstocks, Norwegian oil and gas production, energy from fossil fuels. Oil refining, oil products, refinery design and selected processes, catalytic reforming and isomerization, hydrotreating and hydrocracking, catalytic cracking, treatment of heavy oils, 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. Brief introduction to biomass as the feedstock for biofuels and chemicals, carbon capture and utilization (CCU).

### **Teaching form:**

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, 2<sup>nd</sup> edition, 2013, and articles and handouts.

**Exam:** Written

## TKP4155 Reaction Kinetics and Catalysis

**Responsible:** Professor Magnus Rønning

**Lecturers:** Professor Magnus Rønning

**Semester:** Fall

**Level:** 4th year

**Credits:** 7.5 SP

**Restricted Admission:** No

**Course Plan:** Lectures (4 h/week), exercises (2 h/week), self-study (6 h/week)

### **Objectives:**

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

### **Prerequisites:**

Course TKP4110 Chemical Reaction Engineering or similar knowledge.

### **Contents:**

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

### **Teaching form:**

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

### **Course material:**

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

**Exam:** Written

## **TKP4190 - Fabrication and Applications of Nanomaterials**

**Responsible:** Professor Jens-Petter Andreassen

**Lecturers:** Prof. Edd A. Blekkan, Dr. Sulalit Bandyopadhyay, Dr. Seniz Ucar

**Semester:** Spring

**Level:** 3/4th year.

**Credits:** 7.5 SP

**Restricted Admission:** No

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

### **Objective:**

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

### **Prerequisites:**

Basis chemistry and mathematics and course TMT4320 Nanomaterials.

### **Contents:**

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

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

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

### **Teaching:**

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

## **Catalysis and petrochemistry MSc specialization**

**Coordinator:** Professor Edd Anders Blekkan

### **Course description:**

The specialization involves the following modules:

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

TKP4580 - Catalysis and Petrochemistry, Specialization Project 15 SP

TKP4581 - Catalysis and Petrochemistry, Specialization Course 7.5 SP

Module 1 (KAT) Heterogeneous catalysis. Advanced course 3.75 SP

Module 2 (KEM) Energy and environmental catalysis 3.75 SP

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

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

**Responsible:** Engineer Karin W. Dragsten, Professor Hilde J. Venvik

**Credits:** The course is compulsory and a part of the TKP specialization in catalysis.

**Prerequisites:** None

### **Course description:**

The course is for 5th year students and new Ph.D. students, and is held in the beginning of the autumn semester. The goal of the course is

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

**Teaching methods:** Seminars

**Course material:** Handouts

### **TKP4515-1 Heterogeneous catalysis, advanced course**

**Responsible:** Professor Edd Anders Blekkan

**Credits:** 3.75 SP

**Prerequisites:**

TKP4155 Reaction kinetics and catalysis or similar knowledge.

**Module description:**

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

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

**Course material:** Articles and excerpts from textbooks.

**Language:** English

### **KP4515-2 Environmental and energy catalysis**

**Responsible:** Professor Hilde J. Venvik

**Credits:** 3.75 SP

**Prerequisites:**

TKP4155 Reaction kinetics and catalysis or equivalent knowledge

**Module description:**

Catalysis occupies an important position within areas such as environmental technology and energy production. Within environmental technology catalysis has become crucial not only for removing of unwanted components such as NOX, sulfur etc., but also for the development of selective processes. The course will give the fundamentals for catalytic processes for purification of exhaust gases (NOX, CO, unburned hydrocarbons etc). Within energy production the focus is on biofuel production, catalytic combustion, production of H<sub>2</sub> and catalysis/reactor technology related to fuel cells. Catalysis for clean production will also be an important part of the course.

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

**Course material:** Articles and excerpts from textbooks.

**Language:** English

## Ph.D. courses

### KP8132 Applied heterogeneous catalysis

**Responsible:** Professor Hilde Venvik

**Credits:** 7.5 SP

**Prerequisites:** TKP4155 Reaction kinetics and catalysis.

**Course description:**

The course is given every second year, next time in the fall term 2017.

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

**Teaching methods:** Seminars.

**Course material:** Selected articles and handouts.

### KP8133 Characterization of heterogeneous catalysts

**Responsible:** Professor Magnus Rønning

**Credits:** 7.5 SP

**Course description:**

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

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

**Course material:** Selected scientific papers.



## **KP8136 - Modelling of Catalytic Reactions**

**Responsible:** Professor De Chen

**Credits:** 7.5 SP

**Prerequisites:** TKP4155 Reaction kinetics and catalysis.

### **Course description:**

The course is given every second year, next time in spring 2018

The course gives an overview on the methods for building microkinetic model, collecting or theoretically estimating rate constant, and microkinetic simulation. Focus will also on the microkinetic analysis of reaction systems at the atomic level. A project work of microkinetic modeling of a selected reaction system will be included in the course.

**Learning methods and activities:** Seminars + project

### **Course materials:**

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

## Publications in 2018

1. Chen, Qingjun; Svenum, Ingeborg-Helene; Gavrilovic, Ljubisa; Chen, De; Blekkan, Edd Anders. *Effect of trace potassium on hydrogen adsorption and dissociation on hcp cobalt: A density functional theory study*. Surface Science 2018; Volum 681. s. 24-31
2. Gavrilovic, Ljubisa; Brandin, Jan; Holmen, Anders; Venvik, Hilde Johnsen; Myrstad, Rune; Blekkan, Edd Anders. *Deactivation of Co-based Fischer-Tropsch Catalyst by Aerosol Deposition of Potassium Salts*. Industrial & Engineering Chemistry Research 2018; Volum 57.(6) s. 1935-1942
3. Gavrilovic, Ljubisa; Brandin, Jan; Holmen, Anders; Venvik, Hilde Johnsen; Myrstad, Rune; Blekkan, Edd Anders. *Fischer-Tropsch synthesis—Investigation of the deactivation of a Co catalyst by exposure to aerosol particles of potassium salt*. Applied Catalysis B: Environmental 2018; Volum 230. s. 203-209
4. Patanou, Eleni; Tsakoumis, Nikolaos; Myrstad, Rune; Blekkan, Edd Anders. *The impact of sequential H<sub>2</sub>-CO-H<sub>2</sub> activation treatment on the structure and performance of cobalt based catalysts for the Fischer-Tropsch synthesis*. Applied Catalysis A : General 2018; Volum 549. s. 280-288.
5. Tsakoumis, Nikolaos; Patanou, Eleni; Lögdberg, Sara; Johnsen, Rune; Myrstad, Rune; Van Beek, Wouter; Rytter, Erling; Blekkan, Edd Anders. *Structure-performance relationships on Co based Fischer-Tropsch synthesis catalysts: The more defect free, the better*. ACS Catalysis 2018; Volum 9. s. 511-520
6. Østbye Pedersen, Eirik; Blekkan, Edd Anders. *Noble Metal Promoted CoMn Catalysts for Fischer-Tropsch Synthesis*. Catalysis Letters 2018; Volum 148.(4) s. 1027-1034
7. Østbye Pedersen, Eirik; Svenum, Ingeborg-Helene; Blekkan, Edd Anders. *Mn promoted Co catalysts for Fischer-Tropsch production of light olefins – An experimental and theoretical study*. Journal of Catalysis 2018; Volum 361. s. 23-32
8. Chen, Bingxu; Wang, Di; Duan, Xuezhi; Liu, Wei; Li, Yefei; Qian, Gang; Yuan, Weikang; Holmen, Anders; Zhou, Xingguo; Chen, De. *Charge-Tuned CO Activation over a  $\chi$ -Fe<sub>5</sub>C<sub>2</sub> Fischer-Tropsch Catalyst*. ACS Catalysis 2018 ;Volum 8.(4) s. 2709-2714
9. Chen, Bingxu; Zhang, Xinxin; Wenyao, Chen; Wang, Di; Song, Nan; Qian, Gang; Duan, Xuezhi; Yang, Jia; Chen, De; Yuan, Wei-kang; Zhou, Xingguo. *Tailoring of Fe/MnK-CNTs Composite Catalysts for the Fischer-Tropsch Synthesis of Lower Olefins from Syngas*. Industrial & Engineering Chemistry Research 2018 ;Volum 57 (34) s. 11554-11560
10. Chen, Wenyao; Wang, Zijun; Duan, Xuezhi; Qian, Gang; Chen, De; Zhou, Xingguo. *Structural and kinetic insights into Pt/CNT catalysts during hydrogen generation from ammonia borane*. Chemical Engineering Science 2018 ;Volum 192. s. 1242-1251
11. Cheng, Hongye; Kvande, Ingvar; Zhu, Yi-An; Hammer, Nina; Rønning, Magnus; Walmsley, John; Li, Ping; Qi, Zhiwen; Zhou, Xing-Gui; Chen, De. *Decoding atomic-level structures of the interface between Pt sub-nanocrystals and nanostructured carbon*. Journal of Physical Chemistry C 2018 ;Volum 122.(13) s. 7166-7178

12. Duan, Xuezhi; Zhang, Yanfang; Pan, Minjian; Dong, Hua; Chen, Bingxu; Ma, Yuanyuan; Qian, Gang; Zhou, Xingguo; Yang, Jia; Chen, De. *SbOx-promoted pt nanoparticles supported on CNTs as catalysts for base-free oxidation of glycerol to dihydroxyacetone*. *AIChE Journal* 2018 ;Volum 64.(11) s. 3979-3987
13. Feng, Xiang; Song, Zhaoning; Liu, Yibin; Chen, Xiaobo; Jin, Xin; Yan, Wenjuan; Yang, Chaohe; Luo, Jun; Zhou, Xingguo; Chen, De. *Manipulating Gold Spatial Location on Titanium Silicalite-1 To Enhance the Catalytic Performance for Direct Propene Epoxidation with H<sub>2</sub> and O<sub>2</sub>*. *ACS Catalysis* 2018; Volum 8.(11) s. 10649-10657
14. Feng, Xiang; Yang, Jia; Duan, Xuezhi; Cao, Yueqiang; Chen, Bingxu; Chen, Wenyao; Lin, Dong; Qian, Gang; Chen, De; Yang, Chaohe; Zhou, Xingguo. *Enhanced Catalytic Performance for Propene Epoxidation with H<sub>2</sub> and O<sub>2</sub> over Bimetallic Au–Ag/Uncalcined Titanium Silicate-1 Catalysts*. *ACS Catalysis* 2018; Volum 8.(9) s. 7799-7808
15. Feng, Xiang; Zhao, Yuhai; Liu, Dakuo; Mo, Yasi; Liu, Yibin; Chen, Xiaobo; Yan, Wenjuan; Jin, Xin; Chen, Bingxu; Duan, Xuezhi; Chen, De; Yang, Chaohe. *Towards high activity of hydrogen production from ammonia borane over efficient non-noble Ni<sub>5</sub>P<sub>4</sub> catalyst*. *International journal of hydrogen energy* 2018; Volum 43.(36) s. 17112-17120
16. Gil Matellanes, Maria Victoria; Rout, Kumar Ranjan; Chen, De. *Production of high pressure pure H<sub>2</sub> by pressure swing sorption enhanced steam reforming (PS-SESR) of byproducts in biorefinery*. *Applied Energy* 2018; Volum 222. s. 595-607
17. Jiang, Hongliang; Lin, Yunxiang; Chen, Bingxu; Zhang, Youkui; Liu, Hengjie; Duan, Xuezhi; Chen, De; Song, Li. *Ternary interfacial superstructure enabling extraordinary hydrogen evolution electrocatalysis*. *Materials Today* 2018 ;Volum 21.(6) s. 602-610
18. Kuang, Wuqi; Lu, Mengke; Yeboah, Isaac; Qian, Gang; Duan, Xuezhi; Yang, Jia; Chen, De; Zhou, Xingguo. *A comprehensive kinetics study on non-isothermal pyrolysis of kerogen from Green River oil shale*. *Chemical Engineering Journal* 2018 s. 1-9
19. Li, Qian; Deng, Yun-Xiang; Zhu, Yi-An; Li, Yang; Sui, Zhi Jun; Chen, De; Yuan, Wei-Kang. *Structural stability of Lanthanum-based oxygen-deficient perovskites in redox catalysis: A density functional theory study*. *Catalysis Today* 2018 s. 1-8
20. Li, Yahao; Liu, Daobin; Gan, Jie; Duan, Xuezhi; Zang, Ketao; Rønning, Magnus; Song, Li; Luo, Jun; Chen, De. *Sustainable and atomically dispersed iron electrocatalysts derived from nitrogen- and phosphorus-modified woody biomass for efficient oxygen reduction*. *Advanced Materials Interfaces* 2018; Volum 6:1801623.(4) s. 1-9
21. Lin, Dong; Feng, Xiang; Wu, Yining; Ding, Baodong; Lu, Teng; Liu, Yibin; Chen, Xiaobo; Chen, De; Yang, Chaohe. *Insights into the synergy between recyclable magnetic Fe<sub>3</sub>O<sub>4</sub> and zeolite for catalytic aquathermolysis of heavy crude oil*. *Applied Surface Science* 2018; Volum 456.(31) s. 140-146
22. Niu, Juntian; Liland, Shirley Elisabeth; Yang, Jia; Rout, Kumar Ranjan; Ran, Jingyu; Chen, De. *Effect of oxide additives on the hydrotalcite derived Ni catalysts for CO<sub>2</sub> reforming of methane*. *Chemical Engineering Journal* 2018 s. 1-12

23. Shan, Yuling; Sui, Zhijun; Zhu, Yian; Zhou, Jinhong; Zhou, Xinggu; Chen, De. *Boosting Size-Selective Hydrogen Combustion in the Presence of Propene Using Controllable Metal Clusters Encapsulated in Zeolite*. *Angewandte Chemie International Edition* 2018; Volum 57.(31) s. 9770-9774
24. Sheng, Nan; Liu, Zhikun; Song, Zhaoning; Lin, Dong; Feng, Xiang; Liu, Yibin; Chen, Xiaobo; Chen, De; Zhou, Xinggu; Yang, Chaohe. *Enhanced stability for propene epoxidation with H<sub>2</sub> and O<sub>2</sub> over wormhole-like hierarchical TS-1 supported Au nanocatalyst*. *Chemical Engineering Journal* 2018 s. 1-9
25. Song, Zhaoning; Feng, Xiang; Sheng, Nan; Lin, Dong; Li, Yichuan; Liu, Yibin; Chen, Xiaobo; Chen, De; Zhou, Xinggu; Yang, Chaohe. *Cost-efficient core-shell TS-1/silicalite-1 supported Au catalysts: Towards enhanced stability for propene epoxidation with H<sub>2</sub> and O<sub>2</sub>*. *Chemical Engineering Journal* 2018 s. 1-10
26. Song, Zhaoning; Feng, Xiang; Sheng, Nan; Lin, Dong; Li, Yichuan; Liu, Yibin; Chen, Xiaobo; Zhou, Xinggu; Chen, De; Yang, Chaohe. *Propene epoxidation with H<sub>2</sub> and O<sub>2</sub> on Au/TS-1 catalyst: Cost-effective synthesis of small-sized mesoporous TS-1 and its unique performance*. *Catalysis Today* 2018 s. 1-8
27. Venvik, Hilde Johnsen; Holmen, Anders; Chen, De; Rytter, Erling; Akporiaye, Duncan. *NGCS 11 Tromsø - 11th Natural Gas Conversion Symposium*. *Catalysis Today* 2018 ;Volum 299. s. 1-1
28. Wang, Haizhi; Sun, Lili; Sui, Zhi Jun; Zhu, Yi-an; Ye, Guanghua; Chen, De; Zhou, Xing-Gui; Yuan, Wei-kang. *Coke Formation on Pt-Sn/Al<sub>2</sub>O<sub>3</sub> Catalyst for Propane Dehydrogenation*. *Industrial & Engineering Chemistry Research* 2018 ;Volum 57.(26) s. 8647-8654
29. Wang, Ya-Lan; Wang, Xin-Xin; Zhu, Yi-An; Zhu, Ka-Ke; Chen, De; Zhou, Xing-Gui. *Shape selectivity in acidic zeolite catalyzed 2-pentene skeletal isomerization from first principles*. *Catalysis Today* 2018 s. 1-9
30. Xiao, Ling; Ma, Fang; Zhu, Yi-An; Sui, Zhi-Jun; Zhou, Jing-Hong; Zhou, Xing-Gui; Chen, De; Yuan, Wei-Kang. *Improved selectivity and coke resistance of core-shell alloy catalysts for propane dehydrogenation from first principles and microkinetic analysis*. *Chemical Engineering Journal* 2018
31. Radstake, Paul; Rønning, Magnus; Holmen, Anders. *Influence of H<sub>2</sub> on the Oxygen-Assisted Dehydrogenation of Ethane over Al<sub>2</sub>O<sub>3</sub>-supported Pt-Sn Catalysts*. *Catalysis Letters* 2018 ;Volum 148.(4) s. 1055-1066
32. Rytter, Erling; Borg, Øyvind; Tsakoumis, Nikolaos; Holmen, Anders. *Water as key to activity and selectivity in Co Fischer-Tropsch synthesis:  $\gamma$ -alumina based structure-performance relationships*. *Journal of Catalysis* 2018 ;Volum 365. s. 334-343
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34. Rytter, Erling; Salman, Ata ul Rauf; Tsakoumis, Nikolaos; Myrstad, Rune; Yang, Jia; Lögdberg, Sara; Holmen, Anders; Rønning, Magnus. *Hydrophobic catalyst support surfaces by silylation of  $\gamma$ -alumina for Co/Re Fischer-Tropsch synthesis*. Catalysis Today 2018; Volum 299. s. 20-27
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## Presentations in 2018

1. Blekkan, Edd Anders; Ma, Jianyu; Rout, Kumar Ranjan; Stavnes, Siri. *Zirconium promoted manganese-based solid sorbents for H<sub>2</sub>S capture*. 10th Int. Conference on Environmental catalysis and 3rd EECAT; 2018-09-22 - 2018-09-26
2. Chytil, Svatopluk; Kure, Milly; Lødeng, Rune; Rout, Kumar Ranjan; Ma, Jianyu; Blekkan, Edd Anders. *Supported manganese sorbents for H<sub>2</sub>S capture*. 25th Int. Symposium on Chemical Reaction Engineering (ISCRE); 2018-05-20 - 2018-05-23
3. Tysseland, Amalie; Vanhaecke, Estelle Marie M.; Svenum, Ingeborg-Helene; Blekkan, Edd Anders; Venvik, Hilde Johnsen. *New approaches to the investigation of carbon formation in the Direct Synthesis of Methylchlorosilanes*. Silicon for the Chemical and Solar Industry XIV; 2018-06-11 - 2018-06-14
4. Østbye Pedersen, Eirik; Svenum, Ingeborg-Helene; Blekkan, Edd Anders. *Mn-promotion of alumina-supported cobalt Fischer-Tropsch catalysts*. 18th Nordic Symposium on Catalysis - NSC2018; 2018-08-26 - 2018-08-28
5. Chen, De. *Fundamental issues in controlling carbon supported catalyst performance*. Carbon for catalysis 2018 China; 2018-03-20 - 2018-03-25
6. Chen, De; Fenes, Endre; Baidoo, Martina Francisca; Rout, Kumar Ranjan; Fuglerud, Terje. *Kinetic analysis of redox cycle reaction and catalyst development*. 4th International Conference on Advanced Complex Inorganic Nanomaterials (ACIN 2018); 2018-07-16 - 2018-07-19
7. Chen, De; Rout, Kumar Ranjan; Fenes, Endre; Baidoo, Martina Francisca; Fuglerud, Terje. *Kinetic Analysis and Design of Catalytic Redox Cycles*. 10th International Conference on Environmental Catalysis; 2018-09-22 - 2018-09-26
8. Chen, De; Rout, Kumar Ranjan; Fenes, Endre; Baidoo, Martina Francisca; Fuglerud, Terje. *Kinetic Aspects in Designing Catalytic Redox Cycles*. 11th National Congress of Environmental Catalysis and Environmental Materials; 2018-07-19 - 2018-07-24
9. Chen, De; Rout, Kumar Ranjan; Fenes, Endre; Martina, Baidoo; Terje, Fuglerud. *Kinetic Aspects in Designing Catalytic Redox Cycles*. 25th International Conference on Chemical Reaction Engineering (ISCRE 25); 2018-05-20 - 2018-05-23
10. Chen, De; Wang, Yalan; Qi, Yanying; Yang, Jia; Duan, Xuezhi. *Catalyst Development from Rational Design and Multidimensional Tune of Electrons*. 7th CAS-TWAS Symposium on Green Technology (GT2018); 2018-07-23 - 2018-07-25
11. Chen, De; Yahao, Li. *Sustainable carbocatalyst with atomically dispersed Fe-N-P-C complex active sites for superior oxygen reduction*. 8th Carbon for Catalysis; 2018-06-26 - 2018-06-29
12. Fenes, Endre; Baidoo, Martina Francisca; Ma, Hongfei; Rout, Kumar Ranjan; Fuglerud, Terje; Chen, De. *Descriptors for Alkali Metal Promotion in Redox Catalysis: Ethylene Oxychlorination*. 25th International Conference on Chemical Reaction Engineering; 2018-05-20 - 2018-05-23

13. Fenes, Endre; Ma, Hongfei; Rout, Kumar Ranjan; Fuglerud, Terje; Chen, De. *Calcined Al-Mg Hydrotalcite as Support in CuCl<sub>2</sub> Based Oxychlorination Catalysts*. 18th Nordic Symposium on Catalysis; 2018-08-26 - 2018-08-28
14. Liland, Shirley Elisabeth Sjø; Rout, Kumar Ranjan; Chen, De. *Operando study: Oxidation of Ni-Co/HT Catalyst for Catalytic Combustion of Methane*. 18th Nordic Symposium on Catalysis; 2018-08-26 - 2018-08-28
15. Liland, Shirley Elisabeth Sjø; Rout, Kumar Ranjan; Yang, Jia; Chen, De. *Rational Design of Ni-Co/Hydrotalcite Catalyst for Methane Total Combustion*. 25th International Conference on Chemical Reaction Engineering; 2018-05-20 - 2018-05-23
16. Wang, Yalan; Xiao, Ling; Qi, Yanying; Zhu, Yian; Yang, Jia; Xiao, Wende; Chen, De; Holmen, Anders. *Model-aided catalyst prediction for H<sub>2</sub> production from steam reforming through hybrid semiempirical approach*. The 10th International Conference on Environmental Catalysis & the 3rd International Symposium on Catalytic Science and Technology in Sustainable Energy and Environment; 2018-09-22 - 2018-09-26
17. Yeboah, Isaac; Feng, Xiang; Rout, Kumar Ranjan; Chen, De. *Simultaneously enhanced yield and purity of aviation fuel derived from biomass-derived light oxygenates by one-pot cascade reactions*. The 10th International Conference on Environmental Catalysis & the 3rd International Symposium on Catalytic Science and Technology in Sustainable energy and Environment; (ICEC&EECAT); 2018-09-22 - 2018-09-26
18. Yeboah, Isaac; Rout, Kumar Ranjan; Feng, Xiang; Fan, G; van der Wijst, Cornelis Gerardus; Li, Suizhong; Chen, De. *Insight into Catalytic In-Situ Co/Pyrolysis of Biomass Powder and Bio-Oil as Hydrogen Donor to Green Aromatics*. 26TH European Biomass Conference & Exhibition, EUBCE; 2018-05-14 - 2018-05-17
19. Yeboah, Isaac; Rout, Kumar Ranjan; Yang, Jia; Chen, De. *Valorization of light Oxygenates in Bio-Oil via Catalytic Tandem reaction involving C-C bond Formation*. European Biomass Conference and Exhibition, EUBCE; 2018-05-14 - 2018-05-19
20. Rout, Kumar Ranjan; Yeboah, Isaac; Chen, De. *Tandem catalytic upgrading of simulated bio oil to Jet fuel range aromatics: effects of upstream catalyst*. iCSI seminar; 2018-11-20 - 2018-11-21
52. Ma, Hongfei; Fenes, Endre; Rout, Kumar Ranjan; Fuglerud, Terje; Chen, De. *Mg and K effects on the CuCl<sub>2</sub>/ $\gamma$ -Al<sub>2</sub>O<sub>3</sub> catalyst in ethylene oxychlorination*. Nordic Symposium on Catalysis; 2018-08-26 - 2018-08-28
53. Mahmoodinia, Mehdi; Åstrand, Per-Olof; Chen, De. *Single-atom and Dimer Pt Catalysts Supported by Graphene Nanomaterials: Quantum Chemical Calculations*. Cluster-Surface Interactions Workshop (CSI2018); 2018-06-18 - 2018-06-21
54. Bjørkedal, Ole Håvik; Rønning, Magnus. *One-step sol-gel synthesis of Cu/Ordered Mesoporous Alumina*. Norsk katalysesymposium; 2018-10-16 - 2018-10-17
55. Bjørkedal, Ole Håvik; Rønning, Magnus. *One-step sol-gel synthesis of highly dispersed Cu/Ordered Mesoporous Alumina*. iCSI Annual Seminar; 2018-11-19 - 2018-11-20



56. Regli, Samuel K.; Rønning, Magns. *In situ study of NO oxidation over Pt-based catalysts for nitric acid production*. 6th International Congress on Operando Spectroscopy; 2018-04-15 - 2018-04-19
57. Regli, Samuel K.; Rønning, Magnus. *Operando XRD and XAS study of nitric acid oxidation over supported Pt catalysts*. 17th International Conference on X-Ray Absorption Fine Structure; 2018-07-22 - 2018-07-27
58. Rønning, Magnus. *Carbon-based (Fe-Nx-C) ORR catalysts:-What are the requirements for application in PEM fuel cells?*. 8th International Symposium on Carbon for Catalysis, CarboCat-VIII; 2018-06-25 - 2018-06-29
59. Rønning, Magnus. *Synchrotron radiation in catalysis research*. NorScatt Annual Meeting 2018; 2018-05-22 - 2018-05-22
60. Sørli, Guro; Rønning, Magnus; Mathisen, Karina. *Synthesis of hierarchical CuSAPO-34*. NKS landsmøte i kjemi; 2018-10-16 - 2018-10-18
61. Sørli, Guro; Stoian, Dragos; Rønning, Magnus; Mathisen, Karina. *Verification of hierarchical porosity in CuSAPO-34 by In Situ XAS, N<sub>2</sub> adsorption measurements and NO<sub>x</sub> removal*. XAFS'18; 2018-07-22 - 2018-07-27
62. Strømsheim, Marie Døvre; Svenum, Ingeborg-Helene; Farstad, Mari Helene; Weststrate, C. J.; Borg, Anne; Venvik, Hilde Johnsen. *The CO-induced surface reconstruction on Co(11-20)– a combined theoretical and experimental investigation*. ECOSS 34; 2018-08-26 - 2018-08-31
63. Strømsheim, Marie Døvre; Svenum, Ingeborg-Helene; Farstad, Mari Helene; Weststrate, C. J.; Borg, Anne; Venvik, Hilde Johnsen. *The CO-induced surface reconstruction on Co(11-20)-a combined theoretical and experimental investigation*. Norwegian Catalysis Symposium - Landsmøte i kjemi - October 16th-17th 2018; 2018-10-16 - 2018-10-17
64. Svenum, Ingeborg-Helene; Vicinanza, Nicla; Herron, Jeffrey A.; Mavrikakis, Manos; Venvik, Hilde Johnsen. *Effects of Surface Phenomena on the Performance of Pd-Ag Membranes*. Tailored surfaces in operando conditions; 2018-06-11 - 2018-06-14
65. Venvik, Hilde Johnsen. *iCSI – industrial Catalysis Science and Innovation – a Centre for Research-based Innovation (SFI)*. Norsk Kjemisk Selskap - Det 21. Landsmøte i kjemi - Faggruppe for katalyse; 2018-10-16 - 2018-10-17
66. Venvik, Hilde Johnsen. *iCSI – industrial Catalysis Science and Innovation for a competitive and sustainable process industry, a Centre for Research-based innovation granted by the Research Council of Norway for the period 2015-2022*. 1st Silver Formaldehyde Conference; 2018-01-16 - 2018-01-18
67. Venvik, Hilde Johnsen. *Pd alloy and cobalt single crystal surfaces as catalytic model systems*. Seminar at iNANO, Aarhus University; 2018-06-06 - 2018-06-06
68. Hådem, Gaute O.; Mahmoodinia, Mehdi; Svenum, Ingeborg-Helene; Strømsheim, Marie Døvre; Venvik, Hilde Johnsen. *Nanoscale Investigation of Pd<sub>3</sub>Au(100) Single Crystal as a Model System for Hydrogen Separation*. The 2018 eSSSENCE meeting on Multiscale modelling of materials and molecules; 2018-06-11 - 2018-06-13

69. Hådem, Gaute O.; Mahmoodinia, Mehdi; Svenum, Ingeborg-Helene; Strømsheim, Marie Døvre; Venvik, Hilde Johnsen. *Nanoscale Investigations of Pd<sub>3</sub>Au(100) Single Crystal As a Catalyst Model System*. Time, Work and Function: Time-Resolved Synchrotron and Neutron Techniques for Studies of Soft, Biological and Hard Matter (TWF2018); 2018-06-13 - 2018-06-15
70. Lervold, Stine; Arnesen, Kamilla; Beck, Nikolas; Lødeng, Rune; Yang, Jia; Bingen, Kristin; Pedersen, Terje; Venvik, Hilde Johnsen. *Morphology study of electrolytic silver catalyst for partial oxidation of methanol to formaldehyde (MTF)*. 18th Nordic Symposium on Catalysis (NSC); 2018-08-26 - 2018-08-28
71. Strømsheim, Marie Døvre; Farstad, Mari Helene; Svenum, Ingeborg-Helene; Gavrilovic, Ljubisa; Li, Zheshen; Guo, Xiaoyang; Lervold, Stine; Regli, Samuel K.; Borg, Anne; Venvik, Hilde Johnsen. *Co(11-20) single crystal as Fischer-Tropsch catalyst model system*. NorScatt Meeting; 2018-05-22 - 2018-05-22
72. Strømsheim, Marie Døvre; Farstad, Mari Helene; Svenum, Ingeborg-Helene; Weststrate, C. J.; Gavrilovic, Ljubisa; Regli, Samuel K.; Li, Zheshen; Borg, Anne; Venvik, Hilde Johnsen. *The effect of K on the adsorption and decomposition of ethylene on Co(11-20)*. Tailor2018: Tailored surfaces in operando conditions; 2018-06-11 - 2018-06-14
73. Hillestad, Magne; Ostadi, Mohammad; Alamo Serrano, Gonzalo; Rytter, Erling; Austbø, Bjørn; Pharoah, Jon; Burheim, Odne Stokke. *Need for renewable hydrogen in the biomass to liquid process*. International Hydrogen and Fuel Cell conference; 2018-05-14 - 2018-05-15
74. Hillestad, Magne; Ostadi, Mohammad; Alamo Serrano, Gonzalo; Rytter, Erling; Austbø, Bjørn; Pharoah, Jon; Burheim, Odne Stokke. *Boosting the Carbon Efficiency of the Biomass to Liquid Process with Hydrogen from Renewable Power*. 26th European biomass conference and exhibition; 2018-05-14 - 2018-05-17
75. Anders Holmen: *Fischer-Tropsch Synthesis*. Industrial Catalysis Tutorial Session. Invited Lecture, 10<sup>th</sup> International Conference on Environmental Catalysis, September 22-26, 2018, Tianjin, China.
76. Anders Holmen: *Fischer-Tropsch Synthesis*, Invited lecture at East China University of Science & Technology, September 20, 2018, Shanghai, China.

### Popular science contributions

Ole Håvik Bjørkedal: *Korleis verkar katalysatoren i bilen din?* Published Gemini.no, 26.01.18 and forskning.no 27. 01. 2018

## Seminars 2018

**iCSI**

industrial Catalysis Science and Innovation

**sf** Centre for  
Research-based  
Innovation  
The Research Council of Norway

## iCSI Worskshop 2018

On the 4<sup>th</sup> and 5<sup>th</sup> of November 2018 the majority of iCSI students and researcher assembled together with representatives from iCSI industrial partners and had the opportunity to follow a workshop on **"Challenges in Catalysis Research"**. The two-day event had national reach and occurred in Langesund at the Quality Hotel Skjærgården. The event consisted of **invited lectures** on challenges in catalysis research from renowned scientists. Senior catalyst expert Dr. David Waller from Yara International ASA and senior principal scientist Dr. Konrad Herbst

### Challenges in Catalysis Research

**Location:** Quality Hotel Skjærgården, Stathelleveien 35, 3970 Langesund.

Day 1	Monday November the 5 <sup>th</sup>
12:00 – 13:00	<b>Welcome lunch</b>
13:00 – 13:05	Dr. Nikolaos Tsakoumis, ICSI-NTNU "Challenges in catalysis research"
	<b>Session I Examples of Industrial Challenges</b>
13:05 – 13:40	Dr. David Waller, Yara International ASA "Mechanical properties of catalysts"
13:40 – 14:15	Dr. Konrad Herbst, Haldor Topsoe A/S "From lab scale to production scale: development of an Ag/TiO <sub>2</sub> catalyst for synthesis gas purification"
	<b>Session II From lab to theory and vice versa</b>
14:15 – 14:30	Dr. Yanying Qi, ICSI-NTNU "How to bridge the gap between DFT and experimental study"
14:30 – 14:45	Dr. Mehdi Mahmoodinia, NTNU "Challenges in catalysis science and the role of DFT modelling"
14:45 – 15:00	Endre Fenes, ICSI-NTNU "Promoter Effects on Ethylene oxychlorination reaction for CuCl <sub>2</sub> /γ-Al <sub>2</sub> O <sub>3</sub> based catalysts"
15:00 – 15:15	Stine Lervold, ICSI-NTNU "Improving the Performance of Existing Formalin Production Process Technology"
15:15 – 15:30	<b>Coffee Brake</b>
15:30 – 15:45	Dimitrios Pappas, ICSI-UIO "Revealing the Cu Speciation in Zeolites: An Operando Approach"
15:45 – 16:00	Samuel Regli, ICSI-NTNU "Advanced in situ characterization of catalysts for sustainable process industry"
16:00 – 16:15	Karsten KIRSTE, NTNU "Challenges in making a CoFe functionalized APD silica aerogel for NH <sub>3</sub> decomposition"
16:15 – 16:30	Ata ul Rauf Salman, ICSI-NTNU "Catalysts for attaining NO/NO <sub>2</sub> equilibrium"
16:30 – 16:45	Hongfei Ma, ICSI-NTNU "Ethylene oxychlorination: promoter and structure effect"
16:45 – 17:00	Moses Mawanga, ICSI-NTNU "Intrinsic kinetic parameters & mechanism for NO oxidation over Pt/Al <sub>2</sub> O <sub>3</sub> "
20:00	<b>Dinner</b>
22:00	<b>Departure</b>

### Challenges in Catalysis Research

**Location:** INEOS Olefins & Polymers - INOVYN Europe, at Rafnes.

Day 2	Tuesday November the 6 <sup>th</sup>
09:00	Departure for INEOS refinery, Rafnes.
09:30 – 10:00	Welcome coffee and introductory presentations
10:00 – 11:00	Presentation of the site at Rafnes (ethylene plant, VCM and chlorine plant with focus on the VCM plant)
11:00 – 11:30	Lunch
11:30 – 13:30	Tour on the VCM plant
14:00	Departure for TORP Sandefjord airport





This year's iCSI Seminar 2018 was held in the vicinity of Trondheim next to the lake Selbu and at the historic venue of *Selbusjøen Hotel*. For once more, an idyllic location next to a lake was chosen for hosting our annual meeting. In the 19<sup>th</sup> of November 52 *delegates* from industry and academia were mixed on the scientific event sharing experiences and ideas. In the occasion of the announcement of the *2019 Award for Excellence in Natural Gas Conversion* for Professor Unni Olsbye, a small reception was arranged before the start of the main event and indeed we had the honor to host three winners of the Award for Excellence in Natural Gas Conversion gathered on our annual meeting. Unfortunately, only two members of the *Scientific Advisory Committee (SAC)* were present this time with a busy schedule that included plenary lectures on state-of-the-art approaches to catalysis, direct man-to-man interaction with students in personalized meetings and the iCSI board. Apart from the detailed presentations on the recent developments in each industrial innovation area IIA, highlights on the most developed areas IIA5 and IIA4 were presented by PhD student Dimitrios Pappas and Professor De Chen, respectively. Social interaction through common dining, chatting at the lounge and a team building competitions at the local farm close a very successful meeting.

**2018 iCSI Annual Seminar program**

Date: 19-20 November 2018.  
 Venue: Selbusjøen Hotel (<http://selbusjoenhotel.no/>)  
 (25-30 min from Trondheim airport, 60 min. from Trondheim)

<b>Day 0 (Sunday Nov 18)</b>	
Afternoon	SAC/Board arrival and dinner
<b>Day 1 (Monday Nov 19)</b>	
09:00-12:00	Board meeting
12:00	Registration check-in
13:30	Lunch
13:30-14:00	Opening remarks (Chair of the Board, Odd Arne Lundeberg) Status of iCSI (Director, Heide S. Vabnick)
14:00-14:30	SAC presentation 1, Professor Ericsson (ETHZ, UC Berkeley) Synthetic strategies for the incorporation of metal, alloy, and oxide clusters within crystalline frameworks (Abstracts assembled)
14:30-14:30	Coffee break
14:30-15:00 (25 min + Reception)	iCSI Highlights 1, IIA PhD candidate Dimitrios Pappas Co-Building for the Direct Methanol to Methanol Conversion - Streamlining the Surface of Cu Species (Abstracts assembled)
15:00-15:45 (15 min + 10 min)	SAC 2 update without an innovation and linkage creation SAC 1: Aneta Olsbye/Vaska, UC, Tromsø SAC 2: Aneta Olsbye/Cavka/ETHZ SAC 3: Aneta Olsbye/Cavka/ETHZ
16:00-17:00 (7:00-18:00)	Poster session with contributions from iCSI and related projects Parallel: 1-2 SAC Young Researcher Meeting
18:00-18:30	Reception or social activity
18:30-17:00	Dinner

**Day 2 (Tuesday Nov 20)**

09:00-10:00	SAC presentation 2, Professor Gnanaprakasam, Politecnico di Milano Intensification of Ag production by CVD of AgBr and AgCl/Polyacetylene analysis of the reactor performance by combining in situ optical reactor measurements and modeling (Abstracts assembled)
10:00-10:30	Coffee break (SAC/Board Reception)
10:30-11:00	SA 6 update (Aneta Olsbye)   Parallel SAC research meetings (1-4)
11:00-12:00 (15 + 30min)	Recent advances and iCSI contributions in 1. SETHKA's (Fang) 2. SETHKA's (Fang) 3. SETHKA's (Fang)
12:00-12:00	Lunch (SA/SAC Board meeting)
13:00-13:40 (10 min + Reception)	iCSI Highlight 2, IIA Manager Professor De Chen Elastic mapping, synthesis and design of catalytic metal-oxide
13:40-14:30	Innovation from iCSI (Chair of the Board, Odd Arne Lundeberg) Closing remarks (Chair of the Board, Odd Arne Lundeberg)
14:30-15:00	Coffee/Departure reception Re: to Trondheim Airport (16:00) and Trondheim city center of arrival (16:15)

Wellcome!  
 The iCSI Management and administrative team  
 IIA4, IIA5, IIA6 & IIA7

**Prof. Harry Bitter,**

from Wageningen, The Netherlands (Ljubisa's 1st opponent),  
will give a seminar on

Tuesday 2018, April 17; 10:15, in our meeting room:

**Title: Non-noble metal catalysts in biobased  
conversions.**

(Read about his work in Wageningen here, before moving to WUR  
he worked some 15 years in Utrecht with Krijn de Jong.)

Let me know if anyone is interested in discussing their work him,  
and I will make arrangements for that.

Hope to see you all there!

Kind regards

Edd

## Trial Lectures for the PhD degree

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

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

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

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

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

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

Ola Olsvik: *Catalytic membrane reactors*. 1993

Anne Hoff: *Production of i-butene*. 3/10 1993

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

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

Geir Remo Fredriksen: *Catalytic Combustion*, 17/12 1993

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

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

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<sub>2</sub>-C<sub>4</sub>) 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

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<sub>2</sub>*. 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 from natural 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 NO<sub>x</sub> 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<sub>2</sub> 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<sub>2</sub>-C<sub>4</sub> alcohols from synthesis gas*. 3/11 2010.

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

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

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

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

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

Jia Yang: *Carbide, Nitride and mixed oxide as replacements for noble metal catalysts*. 28/11 2011.

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

Kazi Saima Sultana: *Catalytic conversion of CO<sub>2</sub>*. 2011

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

Hassan Jamil Dar: *Compact steam reformers*. 2012.

Eleni Patanou: *Production of light olefins from syngas*. 2012

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

Ilya Gorelkin: *SCR-deNO<sub>x</sub> catalysis: Catalysis and processes for NO<sub>x</sub> 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 deNO<sub>x</sub> chemistry –state of art and recent progress in methodology and mechanistic insight*. 2014

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



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

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

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

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

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

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

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

Marthe Emelie Melandsø Buan: *Photoelectrochemical CO<sub>2</sub> Reduction to Alcohols*. 2017

Ida Hjort: *State of the art and perspectives in catalytic processes for CO<sub>2</sub> conversion into chemicals and fuels*. 2017

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

Yahao Li: *Synthetic fuels – polyoxymethylene dimethyl ethers as bridging technology for the diesel engine*. 8/3 2018.

Ljubisa Gavrilovic: *A critical view on different pathways to convert biomass to chemicals and fuels*. 18/4 2018.

Erik Østbye Pedersen: *Hydrogen production from hydrocarbons vs. water electrolysis: A comparison of capital and operation expenses as a function of electricity and hydrocarbon prices*. 18/6 2018.

## Alumni

### PhD students Catalysis group:

#### **Per Åge Sørum**

*Hydrogenolysis of esters.  
Conversion of metylformiat to  
methanol*

Defense of thesis: 1982  
Current position: Retired from  
Statoil Mongstad

#### **Edd Anders Blekkan.**

*Characterization and pyrolysis of  
heavy oils.*

Defense of thesis: December 1985  
Current position: Professor NTNU.

#### **Dag Schanke.**

*Hydrogenation of CO over  
supported iron catalysts.*

Defense of thesis: October 1986  
Current position: Retired from  
Equinor, Trondheim

#### **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: Equinor, Adjunct  
professor, NTNU

#### **Edvard Bergene**

*Surface characterization of Pt and  
Pt/Rh gauze catalysts.*

Defense of thesis: March 1990  
Current position: Equinor,

#### **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: Equinor,

#### **Anne Hoff**

*CO hydrogenation over cobalt  
Fischer-Tropsch catalysts.*

Defense of thesis: October 1993  
Current position: IKP, NTNU

#### **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: Equinor,

**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: Aker BP,

Trondheim

**Rune Prestvik**

*Characterization of the metal function of a Pt-Re/Al<sub>2</sub>O<sub>3</sub> reforming catalyst.*

Defense of thesis: October 1995

Current position: Equinor,

**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: Equinor,

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: Equinor,

Trondheim

**Mimmi Kjetså**

*Etherification of methanol and iso/n-propanol with C<sub>4</sub>–C<sub>6</sub> olefins on a macroporous acid ion exchange resin catalyst*

Defense of thesis: May 1998

Current position: Equinor, Stjørdal

**De Chen**

*Methanol conversion to light olefins over SAPO-34: Diffusion, coke depositions and shape selective reactions.*

Defense of thesis: 1998

Current position: Professor, NTNU

**Hans Petter Rebo**

*Application of the TEOM reactor for adsorption, diffusion and kinetic studies*

Defense of thesis: March 1999

Current position: Norsk Industri

**Marit Senum Brownrigg**

*Deactivation and regeneration of bifunctional zeolites*

Defense of thesis: August 1999

Current position: Jotun, Sandefjord

**Ketil Firing Hanssen**

*Cobalt Fischer-Tropsch catalysts studied by steady-state and transient kinetic methods*

Defense of thesis: 1999

Current position: Senior engineer, DNV GL

**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: Equinor, Trondheim

**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: CoFounder AS, Trondheim

**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: Equinor, Stavanger

**Leiv Låte**

*Oxygen-assisted conversion of propane over metal and metal oxide catalysts*

Defense of thesis: 2002

Current position: Force Technology, Trondheim

**Petr Steiner**

*Kinetic and deactivation studies of hydrodesulfurization catalysts*

Defense of thesis: December 2002

Current position: Director, Downstream at Stratas Advisors, Hart Energy Consulting, Belgium.

**Bozena Silberova**

*Oxidative dehydrogenation of ethane and propane at short contact time.*

Defense of thesis: January 2003

Current position: Docent, Hogeschool Rotterdam, Netherlands

**Christian Aaserud**

*Model studies of secondary hydrogenation in Fischer-Tropsch synthesis studied by cobalt catalysts.*

Defense of thesis: May 2003.

Current position: Gassco

**Kjetil Hauge**

*Oligomerization of isobutene over solid acid catalysts for production of high octane gasoline*

Defense of thesis: September 2004.

Current position: Equinor,

**Thomas Løften**

*Catalytic isomerisation of light alkanes*

Defense of thesis: December 2004

Current position: Equinor, 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 Equinor, Trondheim.

**Ingrid Aartun**

*Microstructured reactors for hydrogen production.*

Defense of thesis: June 2005

Current position: Equinor, Stavanger

**Sølvi Storsæter**

*Fischer-Tropsch synthesis over cobalt supported cobalt catalysts.*

Defense of thesis: June 2005

Current position: Equinor, Mongstad

**Erlend Bjørgum**

*Methane conversion over mixed metal oxides*

Defense of thesis: January 2006

Current position: Equinor, Mongstad

**Vidar Frøseth**

*A steady-state isotopic transient kinetic study of Co catalysts on different supports.*

Defense of thesis: May 2006

Current position: Equinor, 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 Equinor, Trondheim.

**Espen Standal Wangen**

*Characterisation and pyrolysis of heavy oils*

Defense of thesis: May 2007

Current position: Teacher, Charlottenlund ungdomsskole, Trondheim.

**Hilde Dyrbeck**

*Selective catalytic oxidation of hydrogen and oxygen-assisted conversion of propane*

Defense of thesis: September 2007

Current position: Equinor, Trondheim

**Svatopluk Chytil**

*Platinum supported on mesoporous silica SBA-15: preparation, characterisation and catalytic properties*

Defense of thesis: September 2007

**Ingvar Kvande**

*Carbon nanofiber supported platinum catalysts.*

Defense of thesis: December 2007

Current position: Researcher, Bioforsk Økologisk, Tingvoll

**Hilde Meland**

*Preparation and characterization of Cu- and Pt-based water-gas shift catalysts.*

Defense of thesis: May 2008

Current position: Researcher, SINTEF Trondheim.

**Silje Fosse Håkonsen**

*Oxidative dehydrogenation of ethane at short contact times.*

Defense of thesis: June 2008

Current position: Researcher, SINTEF Oslo

**Bjørn Christian Enger**

*Hydrogen production by catalytic partial oxidation of methane.*

Defense of thesis: December 2008

Current position: Researcher, SINTEF Trondheim

**Nina Hammer**

*Au-TiO<sub>2</sub> 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, Equinor

**Li He**

*Sorption enhanced steam reforming of biomass derived compounds*

Defense of thesis: January 2010

Current position: Post.doc. NTNU

**Sara Boullosa Eiras**

*Comparative study of selected catalysts for methane partial oxidation.*

Defense of thesis: October 2010

Current position: Yara, Porsgrunn

**Hamidreza Bakhtiary**

*Performance assessment of a packed bed microstructured reactor – heat exchanger for methanol synthesis from syngas.*

Defense of thesis: November 2010

Current position: Xodus Group, Oslo

**Xuyen Kim Phan**

*Catalyst formulations for use in microstructured reactors for conversion of synthesis gas to liquids.*

Defense of thesis: January 2011

Current position: WellChem AS

**Fatemeh Hayer**

*Direct Synthesis of Dimethyl Ether in Microstructured Reactors*

Defense of thesis: March 15 2011.

Current position: Aibel, Stavanger

**Shreyas Panduran Rane**

*Relation between Catalyst Properties and Selectivity in Fischer-Tropsch Synthesis*

Defense of thesis: May 2011

**Fan Huang**

*3D Carbon/polyaniline*

*Nanostructures for Energy Storage*

Defense of thesis: August 2011

Current position: Haliburton, Stavanger

**Oana Mihai**

*Partial Oxidation of Methane by Chemical Looping*

Defense of thesis: September 2011

Current position: Post.doc.

Chalmers, Sweden

**Jia Yang**

*A steady-State Isotopic Transient Kinetic Study of Cobalt Catalysts: Mechanistic Insights and Effect of Cobalt Particle Size, Supports and Promoters.*

Defense of thesis: October 2011

Current position: Assoc. Professor, NTNU

**Nikolaos E. Tsakoumis**

*Deactivation of cobalt based Fischer-Tropsch synthesis catalysts*

Defense of thesis: November 2011

Current position: Project coordinator. NTNU

**Kazi Saima Sultana**

*Calcium Based CO<sub>2</sub> Acceptors for Sorption Enhanced Steam Methane Reforming*

Defense of thesis: November 2011

**Navaneethan Muthuswamy**

*Platinum based Catalysts for Methanol Fuel Cells: Metal Clusters and Carbon Supports.*

Defense of thesis: December 2011

Current positions: Post. doc. Aalto University, Finland

**Hassan Jamil Dar**

*Gas Phase Oxidative Dehydrogenation of Ethane, Kinetics and Reactor Simulation*

Defense of thesis: August 2012

**Eleni Patanou**

*Adsorption Microcalorimetry studies on Cobalt Catalysts*

Defense of thesis: September 2012

Current position: Project coordinator. NTNU

**Paul Radstake**

*Dehydrogenation of Ethane over Alumina-Supported Pt-Sn Catalysts*

Defense of thesis: December 2012

Current position: Franzefoss Minerals, Hylla

**Ilya Viktorovich Gorelkin:**

*Concepts and models of the catalytic dehydrogenation of propane.*

Defense of thesis: March 2013

Current position: Siemens, Trondheim

**Tayyaba Noor**

*Sorption Enhanced Water Gas Shift Reaction: Materials and Catalysis.*

Defense of thesis: June 2013

Current position: School of Chemical and Materials Engineering, SCME, NUST, Islamabad, Pakistan

**Ingvild Tronstad**

*Corrosion of Copper and Oxidation of Dielectric Liquids in High Voltage Transformers.*

Defense of thesis: June 2013

Current position: NAMMO Raufoss

**Fengliu Lou**

*Aligned carbon nanotubes@manganese oxide coaxial arrays for lithium ion batteries.*

Defense of thesis: September 2013

Current position: Beyond AS, Stavanger

**Daham Sanjaya Gunawardana Panditha Vidana**

*Carbon formation phenomena and the initial stage of metal dusting*

*corrosion - an experimental investigation*  
Defense of thesis: January 2014  
Current position: Yara, Porsgrunn

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

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

**Georg Voss**  
*Mesostructured alumina and the state of Ni as promotor for Co Fischer-Tropsch synthesis catalysts.*  
Defense of thesis: August 2014  
Current position: REEtec, Porsgrunn

**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 cobalt 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.*  
Defense of thesis: September 1 2015  
Current position: Institute of Marine Research, Bergen

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

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

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

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



**Marthe Emelie Melandsø Buan**  
*Nitrogen-doped Carbon Nanofibers  
for the Oxygen Reduction Reaction*  
Defense of thesis: March 29, 2017  
Current position: Post. doc. Aalto  
University, Finland

**Ida Hjort**  
*Catalysis for electrochemical  
conversion of CO<sub>2</sub> in aqueous  
solutions*  
Defense of thesis: March 31 2017  
Current position: NAMMO, Raufoss

**Marie Døvre Strømsheim**  
*Co{11-20} and Pd<sub>3</sub>Au{100} single  
crystals as catalyst model system.*  
Defense of thesis: Dec. 13, 2017  
Current position: Post.doc. NTNU

**Yahao Li**  
*Sustainable electrocatalysts for  
oxygen reduction reaction. M-N-P  
(M: transition metals) doped  
mesoporous carbon from biomass.*  
Defense of thesis: March 8, 2018.  
Current position: China

**Ljubisa Gavrilovic**  
*Fischer-Tropsch synthesis –  
Influence of aerosol – deposited  
potassium salts on activity and  
selectivity of Co based catalysts.*  
Defense of thesis: April 18, 2018  
Current position: Post.doc. NTNU

**Erik Østbye Pedersen**  
*Mn promotion effects in Co based  
Fischer-Tropsch production of light  
olefins.*  
Defense of thesis: June 18, 2018  
Current position: NAMMO, Raufoss

