Annual Report

2019

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.

KinCat addresses:

Department of Chemical Engineering, NTNU
N-7491 Trondheim, Norway
http://www.ntnu.edu/chemeng/kincat

SINTEF Industry
Kinetics and Catalysis Research group
N-7465 Trondheim, Norway
http://www.sintef.no

This report was edited by:

Anders Holmen anders.holmen@ntnu.no
Karin Wiggen Dragsten karin.w.dragsten@ntnu.no
Torbjørn Gjervan torbjorn.gjervan@sintef.no

Annual Report 2019
KINCAT
Strong Point Centre Kinetics and Catalysis

Contents

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
Adjunct Assoc. Prof. Kumar R. Rout

SFI-coordinator:

Coordinator Anne Hoff (50% from 06.05.19)

Laboratory personnel:

Engineer Karin Wiggen Dragsten (60% from 06.05.2019)
Senior Engineer Estelle Vanhaecke
Senior Engineer Anne Hoff (40% from 06.05 2019)

Doctoral students 2019/2020:

Ata ul Rauf Salman (- dec 2019)
Stine Lervold
Samuel Regli
Muhammad Zubair
Daniel Skodvin
Ole H. Bjørkedal
Martina Cazzolaro
Jianyu Ma
Hongfei Ma
Mario Ernesto Casalegno
Joakim Tafjord
Jibin Antony
Moses Mawanga
Ask Lysne
Dumitrita Spinu
Junbo Yu
Monica Pazos Urrea
Endre Fenes

Postdoctoral fellows/Researchers 2019/2020

Xiaoyang Guo
Yuanwei Zhang
Ainara Moral Larrasoana
Ljubisa Gavrilovic (-March 2020)
Marie Døvre Strømsheim
Zhenping Cai
Mehdi Mahmoodina
Yalan Wang
Balasingam Suresh Kannan
Yanying Qi
Navaneethan Muthuswamy
Nikolaos Tsakoumis

Visitors 2019/2020

Nianjun Hou
Gang Wang
Wenzhao Fu
Hao Zhang
Xiaoli Yang
Weixin Qian

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

Mikael Hammer
Gunn Torill Wikdahl
Christopher Sørmo
Merete Christensen
Erland Strendo
Ketil Torset Helland

SINTEF Industry, Department of Kinetics and Catalysis

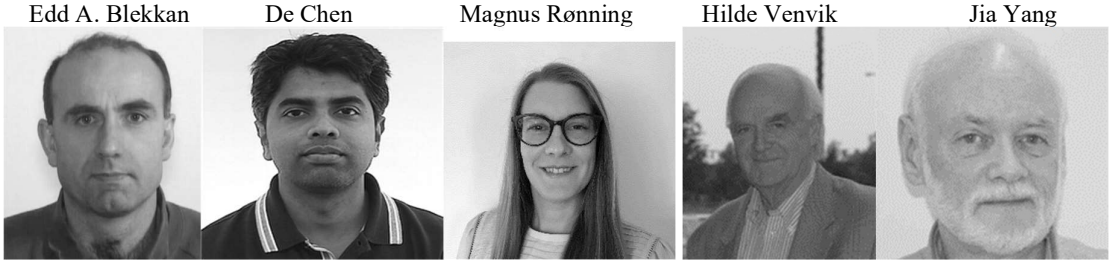
Administration:
Research Manager Torbjørn Gjervan
Senior-/Project Secretary Kirsti Blomsøy

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
Research Scientist Shirley Liland

Laboratory personnel
Senior Engineer Camilla Otterlei

GROUP MEMBERS

Edd A. Blekkan De Chen Magnus Rønning Hilde Venvik Jia Yang

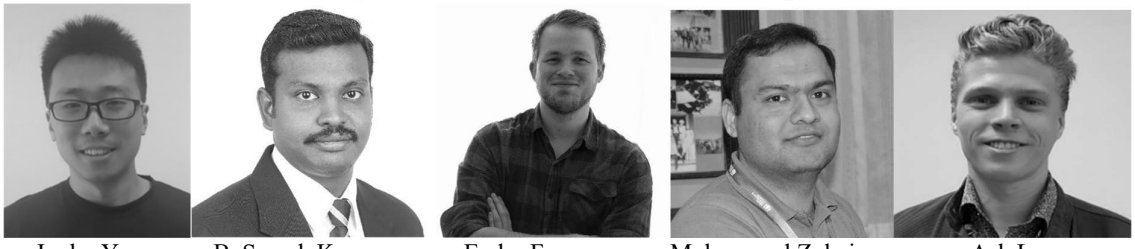


Kjell Moljord Kumar R. Rout Ingeborg-Helene Svenum Anders Holmen Erling Rytter

Karin W. Dragsten Anne Hoff Estelle Vanhaecke Jibin Antony Ole H. Bjørkedal

Mario Casalegno Martina Cazzolaro Stine Lervold Jianyu Ma Hongfei Ma

Moses Mawanga Samuel K. Regli Daniel Skodvin Dumitrita Spinu Joakim Tafjord



Junbo Yu B. Suresh Kannan Endre Fenes Muhammad Zubair Ask Lysne


Mehdi M.


Xiaoyang Guo


Yalan Wang


Ainara Moral


Yanying Qi


Marie Strømsheim

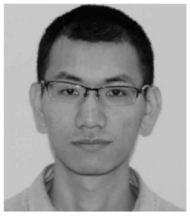
Navaneethan M.


Monica Urrea


Ata ul Rauf S.


Nikos Tsakoumis


Zhenping Cai

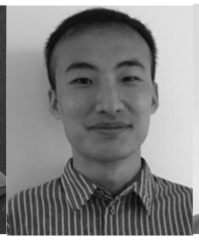

Yuanwei Zhang


Ljubisa Gavrilovic

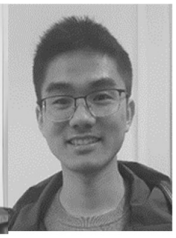

Xiaoli Yang


Nianjun Hou


Weixin Qian


Gang Wang


Wenzhao Fu


Hao Zhang


Håkon Bergem


Hilde Bjørkan


Kirsti Blomsøy


Bjørn C. Enger.


Torbjørn Gjervan


Rune Lødeng


Rune Myrstad


Camilla Otterlei


Kumar R. Rout


Shirley Liland

Research Areas

❖ Conversion of Natural Gas

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

❖ Industrial catalysis

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

❖ Upgrading of Oil Fractions

- Hydrotreating
- Catalytic reforming/isomerization

❖ Biofuels

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

❖ High Temperature Chemistry

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

❖ Environmental Catalysis

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

❖ **Fundamental Studies of Heterogeneous Catalysis**

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

❖ **Microstructured Reactors and Membrane Reactors**

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

❖ **Gas cleaning**

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

❖ **Photocatalysis**

- Water splitting
- Photo reforming
- 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 atm 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 Activities in 2019

- Four candidates completed their PhD degrees in 2019: Issac Yeboah, Yalan Wang, Martina Francisca Baidoo, Ata ul Rauf Salman. The titles of the dissertations, the title of the trial lectures and pictures of the candidates/committees/supervisors are enclosed
- 10 M.Sc. students completed their thesis in 2019. Their name and titles are enclosed. 4 exchange master students also completed their thesis.
- Assoc. prof./Researcher Ingeborg-Helene Svenum has been on a Sabbatical Leave for 2018/2019 in Madison, USA.
- iCSI – industrial Catalysis Science and Innovation – is a Centre for Research-based Innovation (SFI) awarded by the Research Council of Norway (RCN) 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 short description of iCSI is enclosed. The iCSI – Annual Report is available at https://www.ntnu.edu/icsi
- 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 production of biofuels and chemicals from biomass.
- The group is involved in several RCN supported research projects with international collaboration such as EMX2025, GAFT, MBCL, H_2MemX, NanoCat4Fuels.
- The group is coordinating one EU-project and participates in several other EU-projects and networks.
- 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

The 2019 innovation award from the NV Faculty was given to professor **De Chen**. Together with his research group, De Chen has achieved important research results in energy efficient methods for CO_2 capture. They have managed to develop small pellets of natural Norwegian dolomite. These can be reused several thousand times without breaking down or losing the ability to absorb CO_2. This field of research is important for its contributions to decrease climate change - one of our major societal challenges. Through close cooperation with external partners, he has contributed to research impact through innovations. The project has resulted in 7 patent applications during the last two years, as well as interesting spinoff opportunities.

Professor De Chen-Innovator of the year

Hongfei Ma received the best poster award at EuropaCat 14 in Aachen, August 18-23 2019 together with nine others.

The Award for Excellence in Natural Gas Conversion 2019 was given at the NGCS12 meeting in San Antonio to iCSI research partner at the University of Oslo, Professor **Unni Olsbye**.

industrial Catalysis Science and Innovation

for a competitive and sustainable process industry

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

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 that strengthen the industrial value creation and impact the research frontier.

2019 was a year of refreshing the iCSI Centre, with new people joining while others were leaving. First of all, we are proud of the first two iCSI PhDs, Dr Ata ul Rauf Salman and Dr Dimitrios Pappas, who both finalized their degrees in December. They are now in new positions in Norwegian industry, and we wish them success there. We have also welcomed two new PhD candidates to the University of Oslo, Karoline Kvande and Julie Hessevik, and a new Postdoctoral fellow to NTNU, Yalan Wang. All three are well qualified and motivated for their research tasks, and we look forward to following their work in the coming years. Educating master's students is important to the Centre. In 2019, 13 master's students were associated with iCSI, of which five delivered directly into the ongoing projects. The gender balance within iCSI also improved this year, with all personnel categories now balancing – either way – within a 40/60 distribution.

In 2019 our young scientists and senior researchers continued to show their innovation potential by disseminating high quality research from the Centre. iCSI researchers gave 27 presentations at national and international conferences. The number of publications increased from the year before, and 18 reviewed papers were published. At the end of the year, even more were submitted for review.

As announced in 2018, it was an absolute highlight when the Award for Excellence in Natural Gas Conversion 2019 was presented to iCSI professor Unni Olsbye at the 12th Natural Gas Conversion Symposium in San Antonio, Texas in June. She is the first woman to be admitted to this hall of fame in natural gas conversion.

Three iCSI PhD candidates did industrial exchanges in 2019, at Inovyn, Dynea/KA Rasmussen, and Haldor Topsøe. They returned enthusiastic about their new experiences, while also having contributed with new perspectives and skills at the industrial sites.

Due to the midway evaluation workload and the desire to change the season for holding the scientific seminar, iCSI rescheduled the seminar for early summer 2020. This delay was partially compensated by SAC member Enrique Iglesia visiting both NTNU and UiO for full-day meetings with the candidates and other project staff. iCSI appreciated this opportunity to be challenged in inspiring discussions by a man with broad practical experience and a tremendous knowledge within kinetics and catalysis.

Once more the representation on the iCSI Board has changed. Torgeir Lunde, the representative from Yara, replaced Odd-Arne Lorentsen. UiO representative Einar Uggerud (Head of Department of Chemistry) replaced Kristin Vinje, and Marco Piccinini, the representative from Inovyn, replaced Terje Fuglerud. When Odd-Arne left, the Board decided to appoint Pablo Beato from Haldor Topsøe as the new Chair. He has been a Board member from the start-up of iCSI and knows the Centre well. iCSI thanks everyone for their efforts during their period on the Board.

Finally, as the midway evaluation expert panel concluded very favourably for iCSI, and the RCN Board decided that the Centre may continue its efforts, we have started to look forward. We want to learn from our scientific and personal experiences and listen to the advice given to us in the midway evaluation and by our scientific advisory committee (SAC). We continuously work to ensure that we are focusing on the right problems and making optimal use of the unique possibility that we have been given to create innovation through iCSI.

Ph.D. Candidates and Postdoctoral Projects

Advanced biofuels via synthesis gas

Postdoc: Ljubisa Gavrilovic
Supervisor: Edd Anders Blekkan

In this project we have investigated 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. 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 Växjø 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 influences 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:

1. Gavrilovic, Ljubisa; Brandin, Jan; Holmen, Anders; Venvik, Hilde Johnsen; Myrstad, Rune; Blekkan, Edd Anders, The effect of aerosol-deposited ash components on a cobalt-based Fischer–Tropsch catalyst. Reaction Kinetics, Mechanisms and Catalysis 2019, 127, 231-241
2. Gavrilovic, Ljubisa; Save, Jonas; Blekkan, Edd Anders, The Effect of Potassium on Cobalt-Based Fischer– Tropsch Catalysts with Different Cobalt Particle Sizes. Catalysts 2019, 9, 351

Presentations:

1. NGCS - San Antonio 2-6.6.2019 - lecture; Deactivation of the Cobalt Fischer-Tropsch Catalyst - a Kinetic Study, by Ljubisa Gavrilovic, Jan Brandin, Anders Holmen, Hilde Johnsen Venvik, Rune Myrstad, Kumar Ranjan Rout, Erling Rytter, Magne Hillestad, Edd A. Blekkan.

Funding: The Research Council of Norway, contract no. 228741

Bio Fischer-Tropsch - Staging and Multiple Hydrogen Feed of Biomass to Fischer-Tropsch Fuel Synthesis

Project manager and PI for the catalysis activities: Prof. Edd A. Blekkan, NTNU
Postdoc: Ljubisa Gavrilovic
SINTEF Researchers: Kumar Ranjan Rout and Rune Myrstad

The goal of the project is to develop new technology for producing liquid fuels from biomass via gasification and subsequent Fischer-Tropsch synthesis (FTS). FTS is used commercially to convert syngas from coal or natural gas to synthetic hydrocarbons. The liquid products are very well suited to produce aviation fuels and diesel fuel of high quality without sulfur or aromatics. There are, however, many technical and economic challenges that need to be overcome, mainly related to the scale of production and size of the plant. In order to make the process economically viable novel solutions that reduce the investment cost and improve efficiencies are needed. The project is a collaboration between the Catalysis group and the Environmental Engineering and Reactor Technology group at the Chemical Engineering Department at NTNU and the Catalysis group at SINTEF Industry. The idea is to improve the synthesis step by improving the reactor and process technology. The proposed technology has the potential to improve energy- and carbon efficiency of the biomass conversion through the introduction of renewable energy to the gasification step and improved performance of the FTS reaction step. Theoretical and experimental studies of the Fischer-Tropsch synthesis plays a key role in this work. Through the collaborative efforts we will build expertise in fields of high relevance for the utilization of Norwegian lignocellulosic resources for energy and industrial purposes.

Presentations:

1. 27th European Biomass Conference & Exhibition, EUBCE2019, Lisbon, Portugal, 27-31.5.2019; lecture; Modeling, optimization and validation of entrained flow biomass gasifier for syngas production for FT-synthesis, by Koteswara Rao Putta, Kumar Ranjan Rout, Erling Rytter, Edd Anders Blekkan, Magne Hillestad.
2. North American Meeting (NAM26), Chicago 23-28.6.2019 - poster; Modeling Fischer-Tropsch Kinetics for Reactor Design, by Ljubisa Gavrilovic, Anders Runningen, Erik Andreas Jørgensen, Umesh Pandey, Koteswara Rao Putta, Kumar Ranjan Rout, Erling Rytter, Magne Hillestad, Edd A. Blekkan
3. 5th Int. Congress on Catalysis for Biorefineries (CATBIOR 2019), Turku, Finland, 23-27.9.2019, lecture; Modeling Fischer-Tropsch Kinetics for Optimized BTL Plant Design, by Magne Hillestad, Anders Runningen, Kumar Ranjan Rout, Umesh Pandey, Koteswara Rao Putta, Ljubisa Gavrilovic, Erik A. Jørgensen, Erling Rytter, Edd A. Blekkan.
4. Building a sustainable European biofuel industry, Gothenburg, Sweden 4-6.11.2019 - poster; Modeling Fischer-Tropsch kinetics for reactor design, by Ljubisa Gavrilovic, Anders Runningen, Erik Andreas Jørgensen, Umesh Pandey, Koteswara Rao Putta, Kumar Ranjan Rout, Erling Rytter, Magne Hillestad, Edd A. Blekkan.

5. Building a sustainable European biofuel industry, Gothenburg, Sweden 4-6.11.2019 - poster; Optimization of advanced biofuel production via Fischer-Tropsch synthesis, by Umesh Pandey, Koteswara Rao Putta, Ljubisa Gavrilovic, Kumar Ranjan Rout, Erling Rytter, Edd Anders Blekkan, Magne Hillestad.
6. Building a sustainable European biofuel industry, Gothenburg, Sweden 4-6.11.2019 - poster; Kinetic modelling and validation of entrained flow biomass gasifier for syngas production for FT-synthesis, by Koteswara Rao Putta, Kumar Ranjan Rout, Erling Rytter, Edd Anders Blekkan, Magne Hillestad.

Funding: The Research Council of Norway, contract no. 280846

Moving Bed Carbonate Looping (MBCL), Phase 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, Oscar Ivanez, NTNU, Anne Charlotte Gusfre, NTNU

Carbon capture and storage (CCS) has been identified by the International Energy Agency (IEA) as a crucial technology that can be used to meet emission reduction targets (IEA, 2010), as the world transitions to sustainable energy sources. Among the different CCS technologies, the post-combustion CO_2 capture (PCCC) process is the only option for the retrofitting of existing power plants. Furthermore, the CO_2 capture by solid sorbents will diminish the environmental impact of the CO_2 capture and at the same time result in a lower energy penalty in comparison to MEA based PCCC. Carbonation looping using Ca-based oxides has been drawn increasing attention and relatively low energy penalty of the PCCC process. However, the natural Ca-based sorbents suffer a rapid decrease in CO_2 sorption capacity with an increasing number of carbonation/calcination cycles mainly due to sintering and pore closure effects. In order to overcome these problems, Ca-based synthetic sorbents have been developed worldwide. The energy penalty of around 6% points excluding CO_2 compression typically involved in the MEA capture power plant on top of additional CAPEX/OPEX has deterred commercialization of carbon capture and storage so far[1]. To this end, the calcium-looping (CaL) process has attracted great attention from researchers due to its potential to achieve a lower energy penalty than an amine process.

The moving bed carbonate looping concept (MBCL) has been developed by NTNU/SINTEF/FTG since 2017. The philosophy is to reduce the reactor size, cost and energy consumption for post-combustion CO_2 capture by the combined use of process intensification, i.e., by developing optimized process design, cheaper solid sorbents, the compact reactor and easy operation.

A unique reactor design, named Moving Bed Carbonate Looping (MBCL) reactor, has been developed in the current study, as shown in Figure 1. The carbonate looping system, which is arranged downstream, in direction of flow of the combustion exhaust gas (CO_2 rich gas), comprises a moving bed carbonator,

a moving bed calciner and a riser to circulate the CaO solid sorbents. In the carbonator, the solid sorbent flow under gravity in several narrow channels (constrained by gas breathing strainer plates). The combustion exhaust gas goes on cross the sorbent-filled channels, where CO_2 is captured at a temperature of approximately 600°C. The gas also removes heat from the solids due to exothermic carbonation reaction occurs in the channels and the heat removed though HEX outside the channels. Several baffles installed in the carbonator forces the gas passes through the solid sorbents several times before it exits from the carbonator. The calciner section, which is used to regenerate the sorbents, is designed after the same principles. This unique design is capable to handle the large flow of flue gas and keep the solids in the laminar, nearly-plug flow regime. Also, it can reduce the problem related to heat integration and mechanical stability.

In the MBCL Phase II, an attempt is made to increase the TRL of the process design of MBCL concept developed earlier in the MBCL Phase I, with reference to power production of NGCC process. Previously, the heat exchanged between sorbent coming out of carbonator and calciner was done by molten loop and same molten loop was used to provide heat for the calcination from catalytic combustion. But the molten loop is not an advanced technology and several challenges, i.e. corrosion, price etc. occur using the molten loop. Therefore, an alternative design which has high TRL was investigated. The new MBCL process was designed with indirect heat exchange using pressurized combustion flue gas. The pressurized flue gas from the combustion is used to heat exchange between solids from carbonator and calcinator. It is found that the new PCCC power plant has energy efficiency of 55,8%, whereas the energy efficiency of the MBCL phase I was 66.2%. Although the new process design has low energy efficiency, but this removes the risk of molten loop and increases the technical feasibility of the plant. Based on the process design, a complete conceptual design of the moving bed reactor and heat exchanger is done, and it is concluded that the proposed system by a carbonator with a pressurized flue gas from catalytic combustor exchanger is a feasible concept nowadays industrial activity.

Previously, a doped dolomite sorbent was developed stable for ca 200 carbonation and calcination cycles using dry condition and with sorbent possess excellent chemical stability. However, in the real flue gas from the NGCC power plant contains water vapor; thus, it is essential to study the doped dolomite powders in the wet condition. Efforts have been made to study the doped dolomite capture behavior in the wet condition and the sorbent powder possesses excellent capture capacity (above 0.1gCO_2/g-sorbent) and stability for ca 50 carbonation and calcination cycle, which is best-reported data yet. A detailed kinetic study of the developed doped dolomite is done, and a kinetic model is developed, which is used in the reactor modelling. A novel reactor (micro-balance) is developed which simulates the moving bed reactor experiments. A mechanical strength of the

developed doped dolomite is done and found that the solid has enough strength to withstand the plant attrition.

A cold flow pilot unit (Figure 2) has been built in MBCL phase II. The main objective of the bench-scale cold flow reactor was to demonstrate the MBCL reactor concept and study the gas-solid flow behavior of this unique design. Furthermore, a two-fluid reactive CFD model based on the kinetic theory of granular flow (KTGF) are developed. The mathematical model is based on the unsteady, two-dimensional continuity, momentum, energy, and species transport equations. Ansys Fluent software is used to carry out segregated calculations.

Finally, Figure 3 displays the CO_2 concentration distribution in the carbonator. It is clear that CO_2 concentration is decreased as it flows radially across the moving bed.

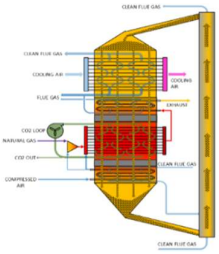


Figure 1. MBCL Reactor design

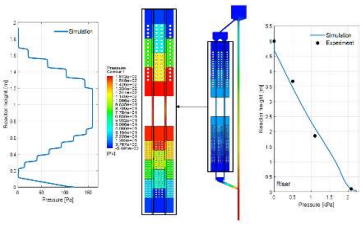


Figure 2. Pressure distribution of the reactor.

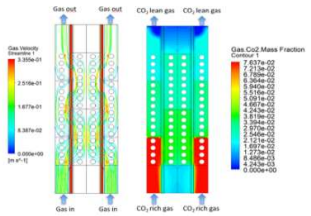


Figure 3. gas stream line (a) and CO_2 concentration (b) in the carbonator.

Presentations:

1. 'Trondheim CCS conference. CO2 capture, Transport and Storage', with a poster presentation titled 'Moving Bed Carbonate Looping (MBCL) Reactor for Post-combustion CO**2** Capture' . Author: Yuanwei Zhang, Kumar R. Rout, Asbjørn Strand, De Chen
2. '26th biennial North American Meeting of the North American Catalysis Society', with a poster presentation titled: 'Kinetic Modelling of CO_2 Capture By Solid Sorbent Based on Ion Migration Hypothesis'**.** Author: Yuanwei Zhang, Kumar R. Rout, Ainara Moral Larrasoana, Li He, De Chen

Financial support: GASSNOVA

Moving Bed Carbonate Looping (MBCL), Phase II

Postdoctoral fellow: Yuanwei Zhang

Supervisors: Prof. De Chen

Giving the increasing fossil fuel consumption and the domination of carbon-intensive industries, carbon capture and storage (CCS) has been identified as one of the most promising technologies for mitigating CO_2 emissions. Among the well-known CCS technologies, the carbonate looping technology has been drawn increasing attention for its low energy penalty.

A unique reactor design, named Moving Bed Carbonate Looping (MBCL) reactor, has been developed in the MBCL project. A cold flow pilot unit has been built at NTNU. In the cold flow experimental study, it has been demonstrated that the plug solid flow can be smooth controlled, and no gas leakage was observed between the carbonator to the calciner.

The MBCL reactor system is a multiphase flow system involving the flow of a dense, reacting, gas–solid mixture with the associated effects of mixing, transport, and mass and heat transfer. A good understanding of the chemical and physical phenomena inside the reactor system is required for the development, optimization, and scale-up of the process. CFD has been widely used for understanding the fluid dynamics and chemical reaction performance of reactors. Hence, detailed CFD simulation is capable for the design and optimization of the reactors while minimizing the need for expensive and time-consuming experimental testing.

A two-fluid reactive CFD model based on the kinetic theory of granular flow (KTGF) has been developed. The mathematical model is based on the unsteady, two-dimensional continuity, momentum, energy, and species transport equations. As evident from the CFD results, good agreement was observed between the predicted and the measured values, indicating the capability of the model for describing the behaviour of the MBCL system. In the future, further simulations will be performed in the MBCL phase **III** in order to accelerate the process of design and optimization of the MBCL reactor.

Financial Support: The MBCL project is financially supported by GASSNOVA

Insights into the kinetics and mechanism of selected industrial catalyzed reactions

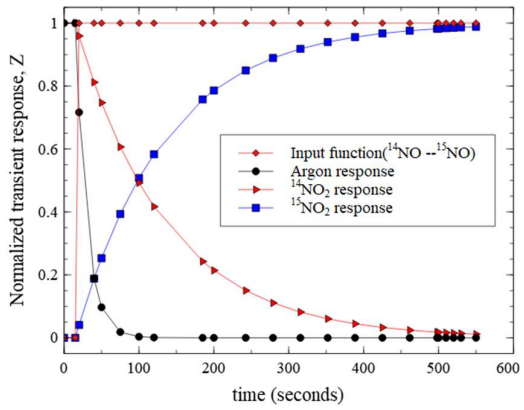
Ph.D. Candidate: Moses Mawanga
Supervisor: Edd Anders Blekkan
Co-supervisor: Jia Yang

Nitric oxide oxidation is a fundamental step in the industrial manufacture of nitric acid. Currently, the NO oxidation process is carried out homogeneously in the gas phase at high NO concentration thus requiring long residence times and efficient heat removal. Knowledge of the kinetics and rate mechanism that accurately describes the catalytic reaction helps to understand the controlling chemical reactions and thereby selecting the reaction conditions that evoke the favorable reaction path over another, thus maximizing the desirable products. It is of great interest to substitute the homogenous oxidation reaction with a heterogeneously catalyzed process to alleviate thermodynamic limitations to have a more intensified process with an added benefit of energy recovery.

The experimental study entails the use of Steady-State Intrinsic Transient Kinetic analysis [1] method coupled with a Diffuse Reflectance Infra-red Fourier Transform Spectrometry (SSITKA-DRIFTS) study on a sample of 1 wt% Pt/Al_2O_3 catalyst prepared by incipient wetness impregnation. Reactant gases constitute primary 10 mol% NO and 6 mol% O_2 in Argon to emulate typical industrial conditions within 150–450 ºC range and atmospheric pressure conditions at a GHSV of 240,000 ml/g_{cat}/h. Upon establishing a steady-state reaction rate, the reactant gas was switched from $^{14}NO + O_2$ to $^{15}NO + O_2$ to study the N-containing pathway as well as $NO + {}^{16}O_2$ to $NO + {}^{18}O_2$ to study the O-containing pathway in the formation rates of $^{14}N^{16}O_2$, $^{15}N^{16}O_2$ as well $N^{16}O^{18}O$, $N^{18}O_2$ products respectively.

The single-pool model [2] was used to analyze the data from the experiments and from this determination of the abundance, surface coverage and the mean residence time (surface lifetime) of reaction intermediates will be estimated. Kinetic Isotope Effects between ^{14}N and ^{15}N as well as ^{16}O and ^{18}O scrambling were ignored. The result is to use this information to discriminate between the dominant mechanism of reaction; either a Langmuir-Hinshelwood type or an Eley-Rideal type as shown in the scheme below, as proposed by [3] and [4] respectively.

Another part of the project involves using adsorption microcalorimetry to measure the heats of adsorption for catalytic activation and functionalization of light alkanes, e.g. using zeolites or metal-exchanged zeolites. 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



Step 1: $O_2 + * \leftrightharpoons O_2*$

Step 2: $O_2* + * \leftrightharpoons 2O*$

Step 3: $O_2* + NO + * \leftrightharpoons O* + NO_2* + *$

Step 4: $2O* \leftrightharpoons O_2^{\nu} + 2*$

Step 5: $2NO + O_2^{\nu} \leftrightharpoons NO_2 + *$

Figure 1. Model for $^{14}NO+O_2$ to $^{15}NO+O_2$ isotopic tracer (left) and an Eley – Rideal reaction scheme for the oxidation reaction (right)

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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.

Advanced characterization of Pd-based membrane model systems

Postdoc: Marie D. Strømsheim
Project organization: Professor Hilde J. Venvik, Research scientist Dr. Ingeborg-Helene Svenum (SINTEF), Senior research scientist Dr. Thijs Peters (SINTEF)

The postdoctoral work is part of the H_2MemX-project, a joint effort between NTNU and SINTEF, and in cooperation with Lund University/the MAXIV Laboratory, to further the understanding of Pd-based membranes for hydrogen separation from gas mixtures. Further knowledge of these membranes is desirable as they may enable the procurement of high purity hydrogen regardless of the feedstock (biomass, natural gas). The specific focus of the postdoctoral project is advanced characterization of the surface chemistry and segregation phenomena of the Pd-alloy membranes/model systems (i.e. single crystals), under as near as possible application conditions. The overall aim is to apply the insight obtained towards optimized membrane performance and stability.
The separation of hydrogen from the other components of the gas mixture occurs through H_2 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 (α→β), 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 and temperatures. Our 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 (polished disk). This patented method allows for easy separation of the membrane from the substrate, as well as control of the thickness and composition of the resulting membranes.
Investigations with ambient photoelectron spectroscopy (APPES) to elucidate the segregation behavior and surface chemistry prior and after exposure to various chemical environments and conditions (C, T, P) of Pd-alloy membranes and model surfaces (single crystals) was carried out at the HIPPIE beamline at MAXIV laboratory. Segregation behavior was studied through repeated cycles of CO oxidation (10:1 O_2:CO), over a $Pd_{75}Ag_{25}$(100) single crystal whilst monitoring the Pd 3d and Ag 3d core levels. Preliminary results show that the segregation was partially reversible, but with the Ag/Pd ratio increasing with the number of CO oxidation cycles. Initial investigations of Pd-23 wt%Ag sputtered, polycrystalline membranes under hydrogen permeation were realized through the design of a reaction cell in collaboration with the MAX IV Laboratory in Lund, Sweden. This cell allowed in-situ characterization of Pd 3d and Ag 3d core levels with APPES of the feed/retentate side of the membranes, with exposure to H_2 in the mbar-range and vacuum on the permeate side.

Acknowledgment:
We gratefully acknowledge the role of MAX IV, in particularly Dr. Jan Knudsen, Dr. Andrey Shavorskiy, Dr. Suyun Zhu of the HIPPIE beamline in the development of the cell and experimental setup, and the workshop at MAX IV for manufacturing parts. The mechanical workshop at the Faculty of Natural Science, NTNU, and the workshop at the Department of Chemical Engineering are also gratefully acknowledged in manufacturing the cell. Virginia Boix (Lund University) and Dr. Mehdi Mahmoodinia (NTNU) are thanked for assisting with the beamline experiments.

Conference contribution:
Strømsheim, Marie Døvre; Svenum, Ingeborg-Helene; Mahmoodinia, Mehdi; Boix, Virginia; Knudsen, Jan; Venvik, Hilde Johnsen. *Investigations of the surface dynamics of Pd-alloy surfaces under oxidation reactions*. 6th annual APXPS Workshop; 2019-12-10 - 2019-12-13

Financial support: The H_2MemX (Enabling ultrathin Pd based membranes through surface chemistry diagnostics and control) project is funded by the Research council of Norway ENERGIX program (grant 280903).

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 Per Erik Vullum, and Dr. Estelle Vanhaecke
Innovation support: Dr Li He

Fe, Ni and Co are known as catalysts for producing carbon nanotubes and carbon nanofibers due to their ability to activate gaseous carbon-containing molecules to form carbon-carbon bonds. In the petrochemical industries, metals and alloys are typically exposed to carbon-saturated gaseous environments with low partial pressures of oxygen and/or steam in a critical temperature range of 400–900 ˚C. Fe and Ni are also main constituent elements of common industrial alloys with desirable high temperature stability. Equipment based on these alloys is therefore susceptible to so-called metal dusting corrosion; a degradation phenomenon that proceeds by a gradual breakdown of the material into a powdery mixture of graphite, carbide and metal particles. Metal dusting carries significant cost since considerable measures are needed in order to avoid catastrophic events in industrial operation.

Pre-oxidized, Ni-based Inconel 601 samples were subjected to carburizing gaseous environments at 750˚C, and carbon formation and surface oxide layer development were investigated by SEM and optical microscopy, AES and Raman spectroscopy. Thin (S)TEM/EDS cross-section lamellae were prepared by Focussed Ion Beam milling. Beyond the initial induction period, less carbon is formed under 10% CO/Ar than under synthesis gas with finite low carbon activity. Cr_2O_3 evolves as a thin surface oxide layer with only CO reacting and more ordered carbon develops with increasing exposure time. In contrast, oxidation yields $(Ni, Fe, Cr)_3O_4$ spinel formation while the materializing carbon remains its disorder during prolonged exposure to synthesis gas. The metal dusting corrosion rate is hence lowered due to Cr_2O_3 stabilization, while the spinel represents an unstable redox state that yields continuous nu carbon. A fine-grained alloy surface structure is also found beneficial to the Cr_2O_3 formation.

The initial stages of carbon formation and metal dusting corrosion of Fe-based Incoloy 800 alloy were studied by SEM, FIB/TEM coupled with EDX/EELS and Raman spectroscopy. The results show that region on the Incoloy 800 samples treated by combined near surface severe plastic deformation (NS-SPD) and consecutive oxidization at elevated temperature exhibit no carbon formation, compared with the region not treated by NS-SPD on the same samples. The good corrosion resistance performance is a result of the NS-SPD process producing an ultrafine-grained structure with a higher fraction of grain boundaries together with crystal twinning near the surface. These microstructures increase the effective

diffusion coefficient for Cr in the alloy by introducing a higher density of rapid diffusion paths, hence promoting the formation of a thin, protective Cr-rich oxide scale during the thermal treatment, which prevents contact between the carburizing atmosphere and the Fe and Ni contained in the alloy. The results imply that the metal dusting resistance performance of Incoloy 800 in industrial applications can be significantly improved by NS-SPD followed by thermal-oxidative treatment.
Our team is selected for European Institute of Innovation & Technology (EIT) Raw Materials Accelerator Program. Funding of 15,000 Euro was granted to improve the market entry success rate of our team, focusing on addressing market risk.

Patents, publications:
Method for reducing metal-dusting corrosion Patent application number 1913256.2 United Kindom Intellectual Property Office
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* Catalysis Today under review.
Xiaoyang Guo; Estelle Vanhaecke; Per Erik Vullum; John C. Walmsley; De Chen and Hilde J. Venvik. *Inhibition of Metal Dusting corrosion on Fe-based alloy by combined near surface severe plastic deformation and thermal treatment (thermomechanical processing)* to be submitted.

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

Surface chemistry of sputtered Pd alloy membrane for hydrogen separation

PhD-candidate**:** Junbo Yu

Supervisor: Professor Hilde J. Venvik

Co- Supervisors**:** Associate Professor Ingeborg-Helene Svenum and Senior Scientist Dr. Thijs Peters (SINTEF)

Hydrogen is seen as a future energy carrier because of its high (gravimetric) energy density, zero emission and variety of sources. Due to different production processes, it is necessary to purify the hydrogen up to levels required for the final application, e.g. fuel cells. In fact, from both technical and economical point of view, the hydrogen purification step is a crucial process in the successful implementation of the hydrogen energy system. Pd-based membranes have been proposed as a good option and have received increased attention from industry due to the high hydrogen selectivity, high thermal stability and mechanical resistance. Hydrogen Mem-Tech AS has designed and built a pilot-plant consisting 19 Pd-alloy membranes tubes from SINTEF for H_2 separation on a side

stream of the Equinor Methanol plant at Tjeldbergodden, Norway. Ultra-pure H_2 is produced, while at the same time, CO_2 will be captured and stored.

Typical mixture gases such as CO and CO_2 are found to have effect on membrane performance. CO may decrease hydrogen permeation flux due to (reversible) competitive adsorption, but high CO concentrations may also cause irreversible degradation by carbon deposition. CO_2 has little impact by competitive adsorption, but its total effects on the surface reaction chemistry remain to be understood. NH_3, as a potential C-free energy storage and carrier, should also be taken into consideration. The effect on the membrane performance is unclear and disputed, with both positive and negative effects reported. Therefore, the surface chemistry of Pd alloy membranes under industrial relevant conditions still needs to be studied.

This PhD project mainly focusses on the thermochemical factors critical to separation performance and long-term stability. Thin Pd based membrane (< 5μm) with no defects and bulk contaminants will be fabricated by SINTEF using their unique, patented two-step magneton sputtering technique. Below this thickness range, surface phenomena become controlling for the overall H_2 transport. A well-designed micro-channel configuration is applied to remove gas phase mass transfer limitations. With carefully prepared and designed experiments, the hydrogen permeation and reaction activity as a function of temperature and partial pressure in different gas mixers is systemically investigated. The effect of surface composition and structure will be analyzed with the help of several advanced characterization techniques such as scanning electron microscopy (SEM), atomic force microscopy (AFM), X-ray photoelectron spectroscopy (XPS) and Auger electron spectroscopy (AES).

Financial support: The H_2MemX (Enabling ultrathin Pd based membranes through surface chemistry diagnostics and control) project is funded by the Research council of Norway ENERGIX program (grant 280903).

CLD-Chemical Looping Desulfurization of Raw Syngas from Biomass Gasification by Mn-based Solid Sorbent

PhD candidate**:** Jianyu Ma
Postdoc**.:** Mehdi Mahmoodinia
Supervisors. Edd A. Blekkan, co-supervisor 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. However, it is a complex gas mixture including H_2, CO, CO_2, H_2O, CH_4 , H_2S and other sulfur-containing species, which can corrode downstream equipment, and also poison catalysts used for fuel synthesis. Hence, sulfur removal from gas streams is an important step for utilizing biomass for energy production.
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 biogas by HTSS represents a promising and energy efficient method for gas cleaning. Mn-based solid sorbents are promising candidates for high temperature sulfur removal, due to their unique chemical properties, their abundance and low cost. The aim of the project is to solve the key technological issues and placing this technology within the portfolio of cost-effective sulfur capture technologies.
The research topics include development of chemically- and mechanically stable Mn-based HTSS spherical pellets, and also establishing a kinetic model for sulfurization/de-sulfurization based on a non-catalytic gas-solid reaction mechanism. The work is part of a larger project, in collaboration with SINTEF, where the experimental results will be used for developing a new reactor model, and a process for gas cleaning.

Publications and presentations in 2019:

1. Ma, Jianyu; Mahmoodinia Mehdi; Kumar Ranjan; Sauer, Maximilian; Blekkan, Edd Anders: *Manganese-based solid sorbents for H_2S capture: Molybdenum promotion*. Building a sustainable European biofuel industry, Gothenburg, Sweden 2019-11-04 – 2019-11-06
2. Ma, Jianyu; Mahmoodinia Mehdi; Kumar Ranjan; Sauer, Maximilian; Blekkan, Edd Anders: *Manganese-based solid sorbents for H_2S capture: Theoretical and kinetic study*. Building a sustainable European biofuel industry, Gothenburg, Sweden 2019-11-04 – 2019-11-06
3. Ma, Jianyu; Mahmoodinia Mehdi; Kumar Ranjan; Sauer, Maximilian; Blekkan, Edd Anders: *Investigation of Molybdenum promoted manganese-based solid sorbents for H_2S capture*. 5th International Congress on Catalysis for bio-refineries, 2019; Turku, Finland 2019-09-23 – 2019-09-27
4. Ma, Jianyu; Kumar Ranjan; Sauer, Maximilian; Mahmoodinia Mehdi; Blekkan, Edd Anders: *Investigation of Molybdenum promoted manganese-based solid sorbents for H_2S capture*. The 12th European Congress of Chemical Engineering; Florence, Italy 2019-09-15 – 2019-09-19.
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capture. The 17th International Conference on Clean Energy (ICCE-2019); Shenyang, China 2019-08-09 – 2019-08-12
6. Mahmoodinia Mehdi; Ma, Jianyu; Sauer, Maximilian; Kumar Ranjan; Blekkan, Edd Anders: *Performance of manganese-based solid sorbents for H2S removal: Particle size and promoter effects on* Gold-Bismutite

Funding: The Research Council of Norway, contract no. 267986

Hybrid Catalysts for Photosynthesis of Ammonia

PhD candidate: Jibin Antony
Supervisor: Magnus Rønning
Co-supervisors: Jia Yang, Sulalit Bandyopadhyay

Ammonia is one of the most important chemicals for the industrial production of fertilizers, pharmaceuticals, and many other nitrogenous compounds [1]. The industrial production of ammonia takes place via the Haber-Bosch process, which requires high temperature and pressure (typically 400-500°C and 200 atm), thereby making it an energy intensive process. This accounts for 1-2% of the world's energy consumption and approximately 5% of the world's natural gas production [1]. The current global production of ammonia is estimated to be around 200 million tons per annum, which accounts for more than 1.6% of global CO_2 emissions [2]. This calls for a pressing need for an alternative greener synthesis route for NH_3 production.

The conversion of N_2 to NH_3 in nature at ambient conditions by the nitrogenase enzyme motivates the search for similar sustainable technologies for industrial scale NH_3 production. Photocatalytic ammonia production is one such field gaining popularity owing to the mild reaction conditions at which it allows the reduction of N_2 to NH_3. Bismutite ($Bi_2O_2CO_3$) nanoparticles (NPs) have recently emerged as an important candidate in photocatalysis owing to the alternative $(Bi_2O_2)^{2+}$ and CO_3^{2-} layered anisotropic crystal structure, which leads to an internal static electric field thereby facilitating photoinduced charge separation and transfer [1]. However, these NPs have a relatively wide bandgap (~ 3.15 eV) which limits its performance in the visible region of the solar spectrum. Furthermore, the high stability of the N_2 molecule with a bond strength of 941 $kJmol^{-1}$, makes the activation step of N_2 quite challenging at these conditions [3]. Hence, the development of highly efficient photocatalytic materials with improved light harnessing properties have garnered significant research interest.

Au NPs, owing to their excellent optical properties and localized surface plasmon resonance (LSPR) effect, have emerged as attractive candidates for catalysis and other applications. As a result of the LSPR effect, enhanced field strength of the electromagnetic fields near the surface of Au NPs can be over 500 times larger

than the applied field for structures with sharp edges [4]. This may cause heating of the NPs by just absorbing sunlight, which could in turn activate the molecules bonded to the surface. Hence plasmon enhanced photocatalysis would improve the solar energy collection efficiency of semiconductors and is expected to give better yields of ammonia. Recent work by Xiao *et al.* reported chemical bath deposition of Au NPs on bismutite and studied the same for photocatalytic ammonia synthesis [1]. However, controlling the morphologies of Au NPs is an area that has not yet been explored, and is expected to have a significant effect on the photocatalytic performance.

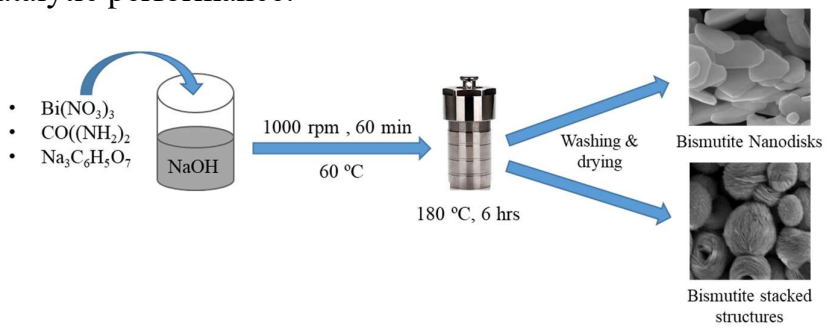

Figure 1 Hydrothermal synthesis route for bismutite NPs

This project aims at synthesizing hybrid NPs of Au with bismutite and to study their performance in photocatalytic ammonia production. Various shapes of bismutite NPs such as disks and 3D stacked structures were synthesized using a facile hydrothermal method as depicted in Figure 1. Au NPs will be deposited on the bismutite NPs via different approaches such as photodeposition, ultrasonication and seed-mediated growth in the presence of cetrimonium bromide (CTAB) as surfactant. The photocatalytic performance of the hybrid catalysts will be studied in the presence of methanol as sacrificial agent under simulated solar light. A 300W Xenon arc lamp equipped with AM1.5 filter will be used to irradiate the reactor under N_2 purging with 1 sun radiation. Careful optimization of the synthesis route for these Au-bismutite hybrids is anticipated to pave way for a greener and energy efficient photosynthesis of ammonia.

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Poster presentations:

1. Antony, Jibin; Oftebro, Kristiane Søvde, Zubair, Muhammad; Bandyopadhyay, Sulalit; Yang, Jia; Rønning, Magnus.(2019) Gold-Bismutite Hybrid Catalysts for Photosynthesis of Ammonia. Nordic Nanolab User Meeting; Copenhagen. 2019.05.07 – 2019.05.08
2. *Sorbent capacity.* Green Energy and Environmental Technology GEET19 Conference (GEET-19), Paris, France, 24.07.2019–26.07.2019.

Enhanced visible light adsorption TiO_2 based catalysts for photocatalytic H_2 production

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

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

Titanium dioxide (TiO_2) is n-type ideal semiconductor photocatalysts, which is being widely used in H_2 production, environmental purification, self-cleaning, CO_2 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_2, it can only absorb UV light up to 380 nm, which is an intrinsic limitation for the TiO_2-based photocatalysts to efficient light harvesting. The charge separation efficiency is a crucial factor for the efficient photocatalytic activity of TiO_2. In spite of its versatility, the mobility of electrons in TiO_2 is low which affects the electron transport rate leading to a decrease in the collection efficiency of the photogenerated electrons. Numerous TiO_2 based photocatalysts have developed for half photocatalytic reaction for H_2 by using the sacrificial reagents by utilizing the photogenerated electrons in the conduction band. These inorganic sacrificial reagents can be easily oxidized to produce different harmful products by the photogenerated holes and promote the H_2 production reaction and making the photocatalytic system expensive. Till the time, there is no such catalysts available with a stat of the art efficiency, selectivity and stability along with the efficient and ideal photoreduction setup.

In this project, to overcome the above-mentioned problem, various approaches like heterojunction formation of TiO_2 with narrow band gap semiconductor, doping of heteroatom, application of co-catalysts will be applied to increase the

photocatalytic activity of semiconductor materials (TiO_2) which are thermally stable, abundance, cost effective and biocompatibility.

Publications and presentations in 2019:

1. Muhammad Zubair, Ingeborg-Helene Svenum, Magnus Rønning, and Jia Yang, Facile synthesis approach for core-shell TiO2–CdS nanoparticles for enhanced photocatalytic H2 generation from water", Catalysis Today, 328 (2019) 15-20.
2. Ata ul Rauf Salman, Signe Marit Hyrve, Samuel Konrad Regli, Muhammad Zubair, Bjørn Christian Enger, Rune Lødeng, David Waller and Magnus Rønning, "Catalytic oxidation of NO over LaCo1-xBxO3 (B =Mn, Ni) perovskites for nitric acid production", catalysts, 9 (2019), 429
3. Muhammad Zubair, Magnus Rønning, and Jia Yang, "Core-shell nanostructures of graphene wrapped CdS nanoparticles and TiO2 (CdS@G@TiO2): The role of graphene in achieving enhanced photocatalytic H2 generation", The Norwegian Catalysis Symposium 2019, 5-6 December 2019, Bergen, Norway
4. Muhammad Zubair, Magnus Rønning, and Jia Yang, "Core-shell nanostructures of graphene wrapped CdS nanoparticles and TiO2 (CdS@G@TiO2)", 1st meeting of the Norwegian NanoSymposium, 16-17 October 2019, Trondheim, Norway
5. Muhammad Zubair, Magnus Rønning, and Jia Yang, "Core-shell nanostructures of graphene wrapped CdS nanoparticles and TiO2 (CdS@G@TiO2) for enhanced photocatalytic H2 generation", European Material Research Society (E-MRS) spring meeting, 26-31 May 2019, Nice, France
6. Muhammad Zubair, Magnus Rønning, and Jia Yang, "Artificial photosynthesis for H2 generation from water employing CdS@TiO2 nanostructures", Norwegian Academy of Technological Sciences, 26 March 2019, Trondheim, Norway.

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

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_2 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.

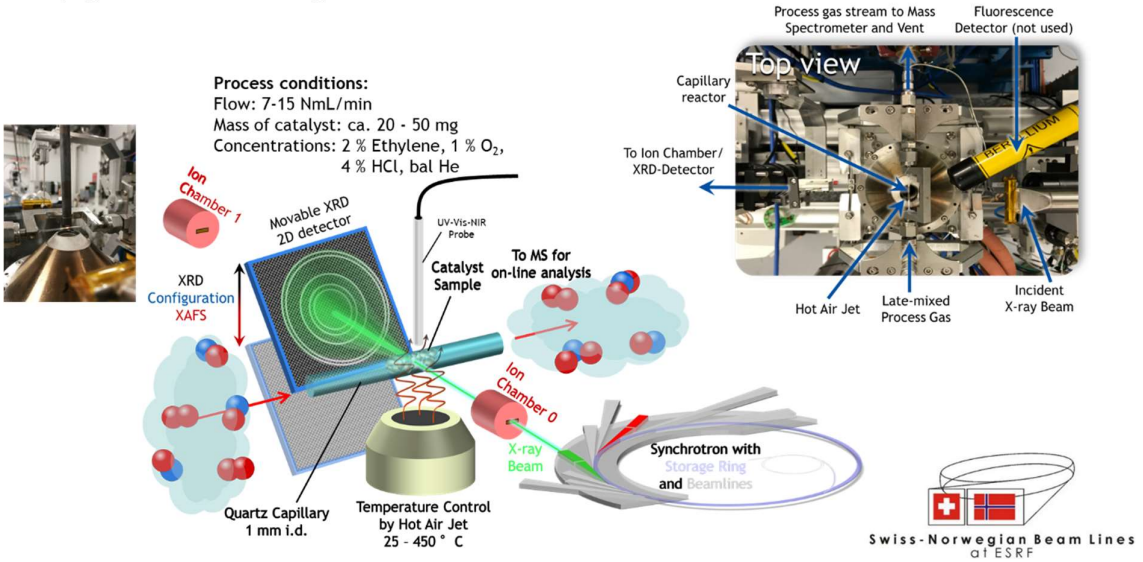

Figure: Experimental Setup for combined operando powder X-ray diffraction and X-ray absorption spectroscopy as well as UV-vis spectroscopy with simultaneous product gas analysis by mass spectrometer at the Swiss-Norwegian Beamlines BM31 at the European Synchrotron Radiation Facility, Grenoble, France

Publications:

Salman AuR, Hyrve SM, Regli SK, Zubair M, Enger BC, Lødeng R, Waller D, Rønning M. *Catalysts*. 2019, 9:429.

Presentations:

1. Regli SK, Salman AuR, Rønning M. Operando X-ray absorption spectroscopy of Pt supported on alumina during catalytic NO oxidation. Operando Surface Catalysis Meeting. Oslo, Norway, 2019-01-29 – 2019-02-01.
2. Regli SK, Fenes E, Ma H, Rout KR, Fuglerud T, Chen D Rønning M. Elucidating Cu species by operando XAS – UV-Vis of CuCl2 Oxychlorination Catalysts. 26th North American Catalysis Society Meeting. Chicago, IL, USA, 2019-06-23 – 2019-06-28.
3. Regli SK, Bjørkedal OH, Rønning M. Operando XAS - UV-Vis of NH3-SCR over highly dispersed Cu catalysts on m-Al2O3. 26th North American Catalysis Society Meeting. Chicago, IL, USA, 2019-06-23 – 2019-06-28.

4. Regli SK, Fenes E, Ma H, Rout KR, Fuglerud T, Chen D Rønning M. Elucidating Cu species by operando XAS – UV-Vis of CuCl2 Oxychlorination Catalysts. EuropaCat 2019, Aachen, Germany. 2019-08-18 – 2019-08-23.

5. Regli SK, Bjørkedal OH, Rønning M. Operando XAS - UV-Vis of NH3-SCR over highly dispersed Cu catalysts on m-Al2O3. EuropaCat 2019, Aachen, Germany. 2019-08-18 – 2019-08-23.

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.

Bio-ethanol steam reforming for on board high purity H_2 generation system

PhD. Candidate: Mario Ernesto Casalegno
Researcher: Nikolaos Tsakoumis
Supervisors: De Chen and 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 H_2 as an energy carrier can be a sustainable solution that will reduce the impact of human activities on the environment. Provided that H_2 is produced in a sustainable way from renewable sources, such as water (using renewable energy) or biomass, it has the potential through its use in fuel cells with favourable efficiencies to cover energy needs with a significant reduction in greenhouse gas emissions. Steam reforming of hydrocarbons is a mature technology for H_2 production. Bioethanol formed by fermentation processes has significant advantages and appears to be a strong candidate as an energy vector suitable for H_2 production.

Our efforts in this project are focusing on the creation of a prototype that integrates steam reforming of bioethanol for H_2 production with CO_2 separation and H_2 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. The optimal process conditions to run experiments will be calculated using Aspen Plus simulator.

Presentations and publications in 2019:

1. M. E. Casalegno, N. E. Tsakoumis, K. R. Rout, E. A. Blekkan and De Chen, Aspen Plus simulations of Steam Ethanol Reforming and promoted Co-Ni/Hydrotalcite structures: Process and catalyst optimization, Oral Presentation, *The Norwegian Catalysis Symposium 2019*, Bergen, Norway, 5 - 6 December.
2. N. E. Tsakoumis, M. E. Casalegno, Y. Wang, E. A. Blekkan, De Chen, Extra pure hydrogen production for mobile applications: An integrated approach, Oral presentation, *NTNU Team Hydrogen Annual Workshop*, Trondheim, Norway 02-03 December 2019.

3. N. E. Tsakoumis, M. E. Casalegno, Y. Wang, K. R. Rout, Y. Zhu, E. A. Blekkan, De Chen, Steam Ethanol Reforming on promoted Co-Ni/Hydrotalcite structures, Poster presentation, 26th NAM, Chicago, Illinois, US, 23-28 June 2019.
4. 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 Catalysis*** 9 (2019) 511–520.
5. N. E. Tsakoumis, E. Patanou, R. Myrstad, E. Rytter, Edd A. Blekkan, Structure-Performance relationships on Co-based Fischer-Tropsch Synthesis: The impact of H2-CO-H2 activation treatment, Oral presentation, 26th NAM, Chicago, Illinois, US, 23-28 June 2019.
6. N. E. Tsakoumis, E. Patanou, R. Myrstad, E. Rytter, Edd A. Blekkan, Structure-Performance relationships on Co-based Fischer-Tropsch Synthesis: The impact of H2-CO-H2 activation treatment, Poster presentation, The 12th NGCS, San Antonio, Texas, US, 2-6 June 2019.

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

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

1,2-propanediol (PD), a major commodity chemical, can be produced via selective hydrogenation of hydroxyacetone (HA): this reaction can be used as a model in the study of selective hydrogenation of carbonyls, that can find application in the upgrading processes of biomass-derived oxygenates streams (i.e. hydro-deoxygenation of bio-oil from biomass pyrolysis, glycerol or products of sugars fractioning). 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 CNF (PCNF) and silica gel (non-carbonaceous reference) were used as supports for catalysts with 5 wt.% Cu loading, prepared by incipient wetness impregnation using Cu

nitrate, acetate or basic carbonate and dissolved in water, ethanol or isopropanol. The catalysts were tested for gas-phase hydrogenation of HA at 240°C and 6 bar. While the Cu precursor showed an impact on activity and selectivity, no important effect of solvent and support was observed. This activity screening needs to be coupled with various characterization techniques to understand the properties controlling the catalyst performance. Furthermore, optimization of catalysts preparation conditions will be explored to tune the Cu-support interaction.

Poster presentations:
Cazzolaro Martina; Yang Jia; Svendby Jørgen; De Clercq Rik; Beier Matthias Josef; Taarning Esben; Chen De. *Stable Cu/C catalysts for selective hydrogenation of hydroxyacetone to propylene glycol.*

- Building a sustainable European biofuel industry. Göteborg, Sweden.
- 14th European Congress on Catalysis, EuropaCat 2019. Aachen, Germany

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

Impact of γ-Al_2O_3 support on ethylene oxychlorination catalyst

Ph.D. candidate: Hongfei Ma
Supervisor: Prof. De Chen
Co-supervisor: Kumar Ranjan Rout & 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, clothe, 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.
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^{2+} and Cu^{+}. Also, by using in situ UV-Vis-NIR spectrometry, reaction rate and Cu^{2+} concentration can be monitored on the operando setups. In this work, two types of γ-Al_2O_3 with tubular- and platelet-like (identified as Al_2O_3-T and Al_2O_3-P

respectively) morphologies were prepared with different methods to have the different facets orientation. Furthermore, these two γ-Al_2O_3 with different morphologies and exposed facets were used as the supports of $CuCl_2$ as the catalyst for ethylene oxychlorination. Herein, we found that the exposed facets of γ-Al_2O_3 have a significant impact on the catalytic activity of ethylene oxychlorination and product selectivity. The catalyst with tubular morphology, with (111) as the mainly exposed facet had a low C_2H_4 conversion, while the one with platelet shape, which was exposed with (110) had a much higher conversion. Moreover, the former is less stable than the latter. The product selectivity was also analyzed, and the results show that more ethyl chloride was formed on the catalyst with tubular morphology γ-Al_2O_3, compared with the catalyst with platelet morphology. Our results confirmed that the supports can have significant influence on both the catalytic activity and product selectivity. The active phase-support interaction is affected by the crystal facets. This finding opens a territory to further understand the support effect in ethylene oxychlorination and the effective modulation of catalyst designing

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[1] N. B. Muddada, U. Olsbye, L. Caccialupi, F. Cavani, G. Leofanti, D. Gianolio, S. Bordiga, C. Lamberti, *Phys. Chem. Chem. Phys.* **12** (2010) 5605.
[2] K. R. Rout, E. Fenes, M. F. Baidoo, R. Abdollahi, T. Fuglerud, D. Chen, *ACS Catal.* **6** (2016) 7030.
[3] D. Gianolio, N. B. Muddada, U. Olsbye, C. Lamberti, *Nuclear Instruments and Methods in Physics Research B* **284** (2012) 53.

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

Promoter effects on $CuCl_2$/γ-Al_2O_3 catalyzed ethylene oxychlorination by DFT calculations

Postdoctoral fellow: Yalan Wang
Supervisor: Prof. De Chen

Ethylene oxychlorination is an important process to produce ethylene dichloride (EDC), which can be used to further manufacture vinyl chloride monomer (VCM) and polyvinyl chloride (PVC). PVC is one of the most commonly used plastic material that has a wide range of applications, such as in households, construction, electronics, pharmaceutical, and automotive industries. Due to the high demand and global increase in demand for PVC, finding efficient catalysts to enhance EDC capacity have a great significance. A large number of catalysts have been developed in the last century for ethylene oxychlorination. Among various catalysts, copper chloride ($CuCl_2$) is identified as a superior catalyst owing to its high activity and selectivity. In addition, γ-Al_2O_3 is recognized as the most commercialized support due to its pore structure, high surface area, high

mechanical strength, high thermal resistance and acidity. However, the $CuCl_2/\gamma$-Al_2O_3 catalyst is prone to deactivation by agglomeration and sublimation of the copper (I) chloride (CuCl) phase. To reduce this phenomenon, promoters are normally added in the $CuCl_2/\gamma$-Al_2O_3 catalyst to maintain and enhance the activity and stability. Although the addition of promoters exhibits better performance, the exact mechanism of the promoter effects remains unclear. In this work, DFT calculations were used to gain insight into the promoter effects and would like to provide some guidance for rational design of catalysts.

The calculations were performed on $3CuCl_2/\gamma$-$Al_2O_3(110)$ with LiCl, NaCl, KCl, RbCl, CsCl, $BeCl_2$, $MgCl_2$, $CaCl_2$, $SrCl_2$, and $BaCl_2$ as promoters, respectively. The formation energy of Cl vacancy was first calculated to probe the ability of removing Cl atoms for $3CuCl_2/\gamma$-$Al_2O_3(110)$ with different promoters. It is found that the addition of CsCl, RbCl, and $SrCl_2$ make Cl vacancy easier to be formed than pure $3CuCl_2/\gamma$-$Al_2O_3(110)$. The analysis of adsorption structures illustrates that all promoters can form bond with $CuCl_2$, which change the electronic properties of $CuCl_2$, and the formation energy of Cl vacancy. The formation energy of Cl vacancy is related to the promoter ionization energy. The locations of active sites are close to that of promoters. Next step, the ethylene adsorption (reduction of $CuCl_2$), the oxygen adsorption (oxidation of CuCl), as well as HCl adsorption (hydrochlorolysis of Cu_2OCl_2) will be calculated to further analyze the promoter effect on reactions.

Publications and presentations in 2019:

1. Y. Wang, H. Wang, A. H. Dam, L. Xiao, Y. Qi, J. Niu, J. Yang, Y. Zhu, A. Holmen, and D. Chen, Catal. Today, 2019, in press, https://doi.org/10.1016/j.cattod.2019.04.040
2. Y. Wang, L. Xiao, Y. Qi, M. Mahmoodinia, X. Feng, J. Yang, Y. Zhu, and D. Chen, Phys. Chem. Chem. Phys., 2019, 21, 19269-19280.
3. Y. Wang, L. Xiao, Y. Qi, Y. Zhu, J. Yang, D. Chen, and A. Holmen, Microkinetic model aided rational catalyst design for light olefins production from synthesis gas through hybrid semi-empirical approach. Poster presentation. North American Catalysis Society Meeting 2019, Chicago, USA. June 23-28, 2019.
4. Y. Wang, L. Xiao, Y. Qi, J. Yang, Y. Zhu, A. Holmen, and D. Chen, Rational catalyst design for Fischer-Tropsch to Olefins by microkinetic modeling through hybrid semi-empirical approach. Short oral presentation. Europacat 2019, Aachen, Germany. August 18-23, 2019.

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

Synthesis of Low Temperature Carbon Dioxide Adsorbents

Ph.D. Candidate: Dumitrita Spinu
Supervisor: Professor De Chen
Co-supervisor: Assoc. Professor Kumar Ranjan Rout

It is well-known that the largest amount of CO_2 emissions comes from fossil fuel power plants, and because of its destructive effect on the global climate, urgent actions must be considered. One of it is CO_2 capture and storage (CCS) which is an intensively researched area aimed at mitigating the CO_2 release into atmosphere. Due to the increase of total natural gas/coal generated electrical power ratio, the project scope is focused on designing CO_2 sorbents for post-combustion natural gas combined cycle (NGCC) power plants. In addition, a cost-effective retrofit can be implemented for the existing power plants.

Various technologies and materials have been developed and investigated, especially the aqueous alkanolamines scrubbing of CO_2. However, the large water content used in this process rises the energy consumption amount, and the direct contact of the amine solution with the equipment requires anti-corrosive materials which are very expensive. Accordingly, amine functionalized solid sorbents are proposed for this project. By anchoring the amine containing material on the pore surface of the support, the amine-equipment contact is avoided. Furthermore, less energy is consumed because no water is involved in the chemisorption process. If comparing with the monoethanolamine NGCC integrated process, a cost saving of 25-30% is estimated by using solid sorbents.

Nevertheless, the amine functionalized solid adsorbents have also some drawbacks like reduced capacity at low CO_2 partial pressure and low chemical and thermal stability. Herein, polyethyleneimine (PEI) and penthaethylenehexamine (PEHA) are planned to be used as the active material for chemisorption. They are described by a very high amine density, an important property required to achieve a high CO_2 adsorption capacity. Moreover, their large molecular weight, especially the one of PEI, increases their resistance to high adsorption-desorption temperatures. However, a very high molecular weight is unwanted because it is difficult to impregnate into the pores. Furthermore, a highly viscous material also involves a very hydrogen bonded environment ($CH_3NH_2 : \cdots H - NH - CH_3$), which minimizes the CO_2 diffusion to the amine sites. The diffusion is also decreased by the high amine loadings. In order to develop large loadings, supports with enough pore volume and pore size are required. In this work, silica supports are used due to their thermal and mechanical stability. The crosslinking and support bonding of amines concepts are also considered in order to avoid amine loss.

The kinetical and performance investigations are already in progress. This year, two master students, Yun Liu and Jørgen Grinna, joined our project. Yun studies the silica supports synthesis method and their physical properties effect on the PEI loading and performance. Jørgen works on the kinetic model of CO_2 adsorption on PEI.

In order to store pure CO_2, the adsorption process should be very selective, and the desorption step should be realized in pure CO_2. As the process is designed based on temperature swing adsorption, a desorption step in pure CO_2 and high temperature deactivate very fast the amines because of the ureas formation.

Secondary amines manifest a quite high resistance towards this type of deactivation, thus a process of converting of primary amines into secondary will be considered. Moreover, the deactivation mechanism will be developed.
The major problem of amine containing materials is their high sensitivity to oxygen. As these materials contain also carbon, the formation of C-O radicals will easily imply the amine group deactivation, especially if the materials or the adsorption environment contain metals like iron or copper, which speed up the radicals' formation. This problem will be tackled in different ways, considering different antioxidants and amine's modifications. Furthermore, the adsorption conditions will be optimized in order to slow down the radicals' formation process.

Presentations in 2019:
Spinu, Dumitrita ; Chen, De ; Rout, Kumar Ranjan. (2019) Lignin to Bio-fuels via Fast Pyrolysis Process Assisted by Volatiles Catalytic Upgrading. Building a sustainable European biofuel industry. Bio4fuels (NO), Supergen Bioenergy (UK), Renewable Transport; Gothenburg. 2019-11-04 – 2019-11-06.

Financial Support: The project is funded by the CLIMIT program in the Norwegian Research Council

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. Anders Holmen and Research Scientist Rune Myrstad

The depletion of oil reserves has increased the interest in developing and improving processes that can replace the use of crude oil. An alternative is the Fischer Tropsch synthesis (FTS), a catalytic process where syngas ($CO+H_2$) reacts to form a range of hydrocarbons, such as light olefins, gasoline, diesel, and waxes. The lower olefins (C_2-C_4) and their derivatives are important building blocks in the chemical industry, 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. This makes iron an attractive catalyst, as it can manage syngas with a relatively wide range of hydrogen content (H_2/CO = 0.5-2.5), due to water-gas-shift activity.

This project focuses on the synthesis of novel Fe-based catalysts. By pyrolysis of Fe-containing polymers, well-dispersed Fe nanoparticles supported on porous carbon are formed. In order to understand how to produce and tailor the best catalysts, an array of synthesis conditions will be explored. The resulting materials

will be investigated with a wide range of characterization techniques to understand how synthesis conditions affect Fe species, particle size and the porosity of the carbon support. In addition to material properties, we will investigate the effect different promoters and activation methods have on the stability, activity, and selectivity during FTS. While the spent catalysts will be characterized, operando studies with XRD and XAS will give valuable information on how different activation methods, promotors, and deactivation affects the catalyst during the reaction. The mechanistic insight will be obtained by Steady-State Isotope Transient Kinetic Analysis (SSITKA) experiments.

Presentations and posters in 2019:
Tafjord, J; Nerb, J; Blekkan, E.A.; Myrstad, R; Holmen, A; Yang, J.
Effect of Potassium on Highly Dispersed Fe-NPs Supported on Carbon for CO hydrogenation. 12th Natural Gas Conversion Symposium, San Antonio. 2019-06-02 to 2019-06-06. Rapid presentation and poster.

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

Low Cost Drill Bit for Geothermal Applications

Researcher: Xiaoyang Guo
Supervisor: Associate Professor: Jia Yang
Co-supervisor: Professor: De Chen

Roller cone drill bits are used in oil & gas wells now 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. This project focused 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. 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. 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.

The wetting ability of SiC by binder alloy is significantly enhanced by improving the synthesis method. Cross-section analysis of the resulting samples after the infiltration test indicates most of the SiC particles are wetted by the binder alloy. Scaling up the synthesis process from 3 g to 100 g shows some issues need to be fixed. Further improvement of the synthesis method in the large scale production is needed.

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

Catalytic Steam Reforming of Hydrocarbons from Biomass Gasification

Ph.D. candidate: Ask Lysne
Supervisor: Prof. Edd A. Blekkan
Co-supervisor: Kumar R. Rout

The growing world population and increasing awareness of the effects of greenhouse gas emissions on the global environment has made the provision of renewable energy sources evident as a major challenge for future sustainable development. The world population is expected to exceed 9 billion people by 2050 and the International Energy Agency (IEA) have estimated a 42-50% increase in the global energy demand by 2035 compared to the 2009 consumption. Renewable energy sources including hydroelectric, wind and solar power can provide vital low-emission electricity, but the electrification of some industrial and transportation niches is limited by the considerably lower energy density and recharging efficiency compared to liquid fuels. The transportation sector accounts for around 25% of the global CO_2 emission, where 90% utilizes petroleum-based fuels. The substitution of currently applied fossil fuels by liquid fuels produced from renewable resources can hereby provide an efficient reduction of the global net CO_2 emission including the considerable advantage of the continued utilization of currently operating combustion engine technology. The annual growth of terrestrial plants stores more than 3 times the global energy demand, and biomass is in practice the only viable feedstock regarding production of renewable carbon-based liquid fuels. The successful adaptation of the Fischer-Tropsch (FT) hydrocarbon synthesis from the original coal to liquid (CTL) technology to the natural gas to liquid (GTL) process has presented the development of biomass to liquid (BTL) and organic waste to liquid (WTL)

technology integrating thermal gasification and FT synthesis as a highly attractive option for high-quality second-generation feedstock liquid biofuel production. The approach includes the considerable advantage of the utilization of already available gasification and FT technology. The successful integration of gasification and FT technology is however limited by technical difficulties regarding the intermediate gas conditioning of the synthesis gas (syngas) requiring the removal of inorganic, organic and particulate contaminants. The elimination of tars has herein been put forth as the most cumbersome challenge of the commercialization of such processes.

The PhD project will address catalytic steam reforming of methane and tars as part of this key gas cleaning step. Initially, the performance of a mixed oxide Co-Ni/Mg(Al)O catalyst prepared from a hydrotalcite precursor will be tested. The effects of Co-Ni ratio and operating parameters like temperature and steam to carbon (S/C) ratio on the steam reforming activity and stability as well as the resistance towards coke formation and sulfur poisoning is within the preliminary scope of the experimental approach.

Financial support: The project is funded through the Centre for Environment-friendly Energy Research (FME) Bio4Fuels.

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

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

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

In this project, the effect of promotors, i.e., mostly alkali, alkali earth and lanthanide elements on turnover frequency, catalytic activity, selectivity and stability is investigated with an operando study, combining mass- and UV-Vis-NIR spectrometry during both transient and steady state experiments.

Two papers are currently close to publication, one combining experimental results and DFT calculations performed by dr. Yanying Qi. Another investigation support effects. The previous year was my last year at the university, and during summer, I left for a new position in the Norwegian petroleum industry. I'm currently attempting to finalize my thesis on my spare time. With the much

appreciated help of my co-authors, I plan to complete the PhD program during the second half of 2020.

Presentations/publications:
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, (under revision)

Financial support: Industrial Catalysis Science and Innovation

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

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

Formaldehyde is the essential component of wood adhesives for a wide range of applications and an important intermediate 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. Parameters affecting the selectivity and stability of Ag will be studied by investigating surface and bulk structural properties and how these develop with time on stream. This approach seeks to identify the effect of reaction conditions on structural properties, applying characterization techniques as XRD, SEM, EBSD and Kr-BET.
Investigation of both chemical and kinetic aspects will be performed in a so-called annular reactor. The annular reactor offers a controlled system with laminar flow, isothermal conditions and potentially negligible mass transport limitations and gas phase reactions. Experimental data obtained will be utilized in a COMSOL model.

Publications and presentations in 2019:
1. 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.* Top Catal 62, 699–711 (2019).

2. Stine Lervold, Kamilla Arnesen, Nikolas Beck, Rune Lødeng, Jia Yang, Kristin Bingen, Johan Skjelstad, Hilde J. Venvik. *Morphology study of electrolytic silver catalyst for reactions relevant to partial oxidation of methanol to formaldehyde (MTF).* 14th European Congress on Catalysis, EuropaCat 2019, Aachen, Germany, 2019. Oral presentation.

Financial support: The project is a research activity (IIA3, WP3.1) under iCSI – industrial Catalysis Science and Innovation for a competitive and sustainable process industry", which is a National Centre for Research-based Innovation (SFI) granted by the Research Council of Norway (Contract number 237922).

Catalysts for NOx-reduction in maritime transportation

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

Stricter regulations for maritime nitrogen oxide (NOx) emissions are expected to create a demand for non-toxic NOx-reduction catalysts able to perform at a wide range of operating conditions with special regards to oxygen content and temperature in the exhaust stream.
Liquefied Natural Gas (LNG) is becoming more attractive as maritime fuel, due to its increasing supply and opportunity for more efficient and cleaner combustion. However, the combustion process is usually performed with surplus oxygen to minimize the risk of methane slip. Such conditions facilitate generation of thermal NOx, which must be reduced downstream of the engine.
The goal of the project is to develop catalysts for Selective Catalytic Reduction (SCR) under relevant conditions for LNG-propelled ships, as well as reaching a better understanding of the role of the support in SCR-catalysis.
High surface area, surface acidity and thermal stability are regarded to be important properties for an SCR-catalyst. Mesoporous alumina (MA) prepared through a sol-gel synthesis may be a way to obtain these properties in a support material. Catalysts with highly dispersed Fe and Cu on an MA-support have been synthesized and characterized by a.o. In-situ XAS/XRD experiments at the Swiss-Norwegian Beamline (SNBL) at ESRF in Grenoble to determine the state of the active metal during the SCR-reaction.
The alumina-supported samples were found to have some interesting material properties such as high dispersion for high loading, but the SCR-activity was fairly low. The synthesis principle has been used to make similar ZrO2-supported Cu and Fe catalysts. These samples appear to have similar material properties and promising SCR-activity.
Lisa Leganger Landfald worked with the project for her master project. She submitted her thesis in February 2019 with the title *Fe-ZSM-5 and Fe-SAPO-34*

Catalysts for Low-Temperature Selective Catalytic Reduction of NOX by NH3. Her work regarded iron-zeolites and zeotypes (Fe-ZSM-5, Fe-SAPO 34), investigating synthesis methods and their influence on SCR performance.

Poster presentations in 2019:
Bjørkedal, Ole Håvik; Regli, Samuel K.; Rønning, Magnus**.** *Cu-containing mesoporous alumina as catalysts for SCR.* Europacat 2019; 2019-08-18 - 2019-08-23 NTNU

Financial support: The project is funded by the Norwegian Research Council through the EmX 2025 program, project 246862

Developing cost-effective Pt-based electrocatalysts supported on CNF for ORR

Exchange Ph.D. Student: Hao Zhang
Supervisors: Prof. De Chen
Co-supervisors: Dr. Navaneethan Muthuswamy

Proton-exchange membrane fuel cells (PEMFC) have showed great prospect in transportation by eliminating the emission of green house gases, but their wide application is limited by the lack of cost-effective cathodic electrocatalysts for ORR. The integration of carbon support and well-designed Pt-based bimetallic nanoparticles is considered as a promising way to solve this problem. In this project, carbon nanofiber (CNF) will be used as support materials due to the combined advantages of electronic conductivity, high surface area and stability. On the other hand, the specific structures of Pt combining with transition metal Co involve intermetallic alloy and core-shell structure, which not only reduces the usage of Pt but also improves the inherent activity of Pt sites under the effect of metal-metal interaction and lattice strain.
Firstly, the single Pt nanoparticles supported on CNF were prepared by an ex-situ colloidal synthesis method. In this method, the size of Pt nanoparticles is controlled in the colloidal solution before depositing on the corresponding supports. Electrochemical measurements were performed in a three-electrode system with a rotating disk glassy carbon electrode connected to a potentiostat. The ORR-activities were determined by performing linear sweep voltammetry (LSV) from 1.1V to 0.01V at a sweep rate of 5mVs-1 in an O2-saturated 0.1 M HClO4 electrolyte, with a rotating speed of 1600 rpm. The ORR mass activity for Pt/pCNF (25 wt%) shows 0.085 A/mgPt at 0.9 V which is much lower than the target (0.44 A/mgPGM) set by DOE for platinum group metal catalysts, but is higher than commercial 30 wt% Pt/C (0.075 A/mgPGM).
In future work, the bimetallic nanoparticles supported on CNF including PtCo alloy and PtCo core-shell structure will be prepared and tested. Characterization including TEM, XPS, EXAFS and XANES will also be done to understand the catalysts behavior for the above electrochemical reactions.

Kinetic Modeling of Redox Catalytic Cycles on Cu-based catalysts for toluene oxidation

Exchange PhD student: Wenzhao Fu
Supervisor: Prof. De Chen
Co-Supervisor: Prof. Jia Yang

Volatile organic compounds (VOCs), emitted from a variety of industrial processes and transportation activities, are considered as an important class of air pollutants. Catalytic oxidation is one of the most developed techniques used for the elimination of VOCs, as it requires lower temperatures than thermal oxidation. Herein, we choose the toluene as VOCs probe molecule because aromatics are present in the industrial and automotive emissions. Typical catalysts for toluene oxidation are mainly noble metals, which have high activity at low temperatures, while they are costly. Metal oxides (Fe, Cr, Cu, Mn and Co) are a cheaper alternative to noble metals as catalysts for VOC oxidation. They present sufficient activity, although they are less active than noble metals
at low temperatures. Cu mixed metal oxides catalysts are effective oxidation catalysts due to their high oxygen storage capacity and facile Cu/Cu^{2+} redox cycle. On the other hand, catalysis is a kinetic phenomenon, the toluene total oxidation reaction is the combination of the reduction and oxidation of the catalysts, and the detail reaction mechanism, as well as its active sites, are not yet fully understand. In the present work, we comparatively studied the toluene oxidation on the Cu/Al_2O_3 and Cu/TiO_2 catalysts to understand the oxygen vacancy dependent reaction activity. Based on our group's previous research, with the help of the in-situ UV-Vis-NIR spectrometry and MS data, the step transient and steady-state operando kinetic studies can provide the exact information of the transformation of Cu species, quantify the change of oxygen vacancies and the corresponding reaction rate. The latest results suggest both the reduction ability of the CuO by toluene and the amount of the oxygen vacancy determining the reaction rate.

Insights into the Kinetics and Mechanism of Propylene Epoxidation with H_2 and O_2

Exchange Ph.D. Candidate: Gang Wang
Supervisor: De Chen
Co-supervisor: Jia Yang

Direct epoxidation of propylene with H_2 and O_2 to produce propylene oxide (PO), which could avoid the environmental and economic issues in the traditional processes, has received considerable attention since it was first reported over titania supported gold catalyst in 1998. Up to date, the low PO formation rate, low H_2 efficiency and poor catalysts stability still limit this route to realize

commercialization. In this research, Au/TS-1 and Au/TiO_2 catalysts with different gold loading were prepared with deposition precipitation method. Catalytic performance test was performed in a fixed bed reactor with UV-vis to monitor the coordination states of Au and Ti sites, and MS to obtain the products distributions. H_2 and O_2 were used to produce hydrogen peroxide to oxidize Ti sites, and C_3H_6 was employed to reduce Ti-OOH species to finish the redox cycle. This could be used to determine the real oxidation states of Au and Ti sites and identify the rate determining step in the propylene epoxidation. On the other hand, in-situ FT-IR was used to probe the adsorbed species on the catalysts surface to investigate the coke formation mechanism. With these fundamental experimental data, it will be possible to have a better understanding of the reaction mechanism and thereby for better catalyst design and optimization.

Carbon materials for ultra-high energy density supercapacitor

Researcher**:** Navaneethan Muthuswamy
Supervisor: Prof. De Chen

Global electric vehicle sales currently are about 1 million per year, and the number is expected to increase more than thirty times by 2030 (Bloomberg New Energy Finance). Most electric vehicles currently use Li-ion batteries to drive the electric motor with power around 100 kW (~ 134 horsepower). Another potential onboard storage device is supercapacitor, which exhibits higher specific power (upto 10,000 W/kg) and better cyclic stability than Li-ion batteries. In addition, supercapacitors can charge and discharge much faster than Li-ion batteries. Supercapacitors are currently used in hybrid electric vehicles for kinetic energy recovery (regenerative braking systems), as they can charge quickly during the braking process by converting mechanical energy to electric energy through a generator. Also, they can discharge very fast to deliver high power in a short period of time to accelerate electric vehicles rapidly. The potential applications for supercapacitors include hybrid buses, marine vessels, speed boat, cranes, mining equipment, backup systems etc.
The main disadvantage of supercapacitors is that the specific energy (~ 4 to 10 Wh/kg) is very low, 100 times lower than the Li-ion battery. This demands for higher unit weight and hinders the use of supercapacitors as a sole energy storage system. The energy density of a supercapacitor is directly proportional to the capacitance times square of the voltage across the unit cell. The voltage window is limited to 3 volts in organic electrolyte. Above this operating voltage the electrolytes decompose at the activated carbon electrode surface due to the presence of defects and surface functional groups. This project aims to widen the operating voltage window of supercapacitors by developing activated carbon with reduced defects and stabilized functional groups. The project is conducted in close collaboration with the Stavanger-based company Beyonder AS.

In the initial stage of the project, the carbon raw materials (the source for carbon activation) were produced in bulk through a novel method developed in the catalysis group at NTNU. The carbon materials are also subjected to different physical activation and post heat treatment processes at different conditions to alter the surface properties. The obtained carbon materials will be tested for supercapacitor performance in coin cells using Tetraethylammonium tetrafluoroborate as electrolyte.
Part of the project is also to demonstrate the possibility for carbon production in bulk and to build a network with academic and industrial partners to find applications for the carbon materials produced through this novel method. This part of the project is funded by NTNU through NTNU discovery. So far, the carbon production has been upscaled from below one gram to above 10 grams. Since the method is very precise in controlling the surface and internal properties of the carbon materials there is a wide scope to utilize them in different applications such as fuel cells, supercapacitors, batteries, air purifiers, coating technologies and in water treatment process.

Financial support: The work is financed by Norwegian Research Council and NTNU through NTNU discovery project.

Catalysts for attaining NO/NO_2 equilibrium

PhD Candidate: Ata ul Rauf Salman
Supervisor: Professor Magnus Rønning,
Co-supervisors: Rune Lødeng, Bjørn Christian Enger (SINTEF), David Waller (Yara)

Nitric acid is a valuable commodity chemical with an annual global production of about 65 million tonnes. Almost 80% of global production is converted to fertilisers, while the remaining is used for the production of nylon, foam, paint, explosives, etc. Wilhelm Ostwald developed and patented the process for production of nitric acid based on catalytic oxidation of ammonia in 1902, and it is exclusively used for all industrial production. The process comprises three important chemical steps: In the first step, ammonia is oxidised with air over Pt/Rh gauzes at elevated temperatures to yield nitric oxide (NO). In the second step, NO is further oxidised to nitrogen dioxide (NO_2) as a homogenous gas-phase reaction. Finally, NO_2 reacts with water in the absorption column to yield nitric acid.
Replacing this homogenous reaction with a more compact heterogeneous catalytic process offers several advantages: a) a significant increase in recovery of high-quality heat b) acceleration of the oxidation reaction and c) potential for a substantial decrease in capital expenditure (CAPEX) for new plants. There have been some efforts to find a catalyst that is effective under industrial conditions,

but to this date, the process is still carried out as a homogeneous reaction in modern nitric acid plants.

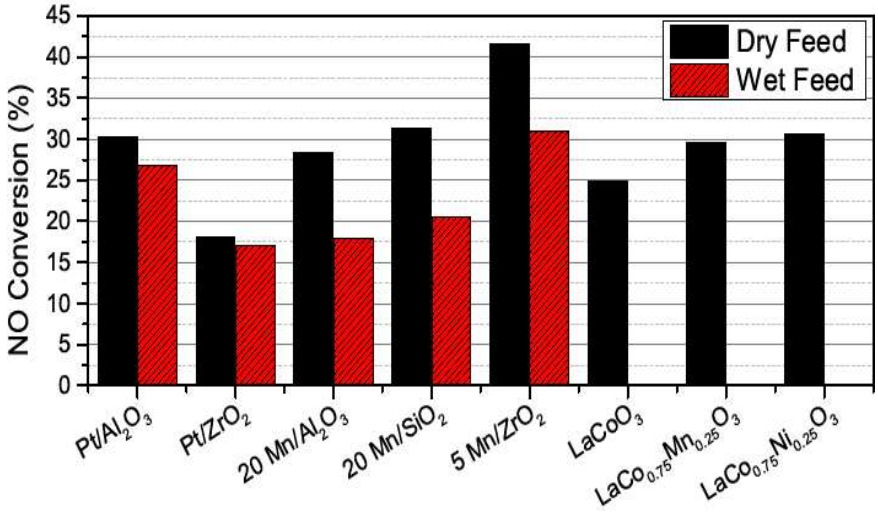

Figure 2: NO Conversion over various catalysts at 350 °C during temperature scan from 150 °C to 450 °C. Feed 10% NO, 6% O_2 (15 % H_2O when present) in balance Ar

The current work is aiming to find efficient catalysts for oxidation of NO to NO_2, at conditions relevant to nitric acid plant, enabling significant process intensification of the production plant. Additionally, the aim was to gain fundamental understanding of reaction kinetics and the mechanism of oxidation of NO over promising catalysts. The industrial process dictates the boundary conditions of catalytic investigations: Feed composition of 10% NO, 6% O_2, 15% H_2O, pressure 1–10 bar and temperatures in the range 150 – 450°C.
Mimicking industrial conditions in a laboratory is challenging. A dedicated setup was built capable of investigating the activity of powdered catalysts using realistic feed concentrations at atmospheric pressure partially simulating nitric acid plant conditions. The activity of the catalysts was studied as a function of temperature to provide information about the onset temperature of catalytic conversion. The stability of the catalysts was probed by studying catalytic activity as a function of time. Although the water is an integral part of the reaction mixture in the nitric acid plant, catalytic experiments were performed in the absence and presence of water to elucidate the effect of water on catalyst activity and structure. The NO conversion levels at 350°C for the various catalysts are presented in Figure 1.
Platinum catalysts supported on Al_2O_3 and ZrO_2 have been investigated for the oxidation of NO. Another primary focus of the project was to identify potential replacements of platinum group metal (PGM) catalysts, exhibiting superior or comparable catalytic activity. Therefore, transition metal oxide (manganese) on different support materials (Al_2O_3, SiO_2, ZrO_2) and perovskites ($LaCo_{1-x}B_xO_3$, B = Mn, Ni) have been investigated. The experimental results revealed that zirconia-supported catalysts with low manganese loading are promising cost-efficient catalysts for the conversion of NO in nitric acid production.

Publications in 2019:

1. Salman AuR, Catalytic oxidation of NO to NO_2 for nitric acid production, PhD Thesis, NTNU 2019
2. Salman AuR, Hyrve SM, Regli SK, Zubair M, Enger BC, Lødeng R, Waller D, Rønning M; Catalytic Oxidation of NO over $LaCo_{1-x}B_xO_3$ (B = Mn, Ni) Perovskites for Nitric Acid Production, Catalysts. 2019, 9:429
3. Salman AuR, Regli SK, Enger BC, Lødeng R, Waller D, Rønning M, Revealing the Structural and Chemical State of Platinum Nanoparticles during Oxidation of NO to NO_2 at Nitric Acid Plant Conditions, 26th North American Catalysis Society Meeting, Chicago, IL, USA, 2019-06-23 – 2019-06-28

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

Design of nitrogen-doped carbon materials for oxygen reduction reaction

Ph.D. Candidate.: Nianjun Hou
Supervisor: Professor De Chen

Fuel cells are considered as a promising replacement of traditional energy solutions in terms of providing clean, steady and sustainable power to meet the rising global energy demand. H_2 is oxidized at the anode while O_2 is reduced at the cathode, and current flows through the circuit. A hydrogen fuel cell can work under alkaline or acidic conditions. The oxygen reduction reaction (ORR) has much slower kinetics compared with the hydrogen oxidation reaction in both media. The performances and costs of fuel cells therefore largely depend on the ORR electrocatalysts used.

Pt and its alloy established high activity, which are heavily studied and often chosen as benchmark materials. However, as one of the noble metals, Pt is too expensive, easy to be poisoned and has poor selectivity. The cheapest catalysts are carbon-based catalysts. These catalysts possess comparable activities and high selectivity. They also stable in most electrolytes.

In this research, polymer derived carbon nanospheres are synthesized and used as efficient ORR catalysts. The N content could be tuned by using different precursors. The BET surface area, pore size distribution and pore volume could be optimized by a careful study of the activation procedure with ammonia. Furthermore, Fe, P, Cl could also be introduced to improve the performance of the catalyst.

To date, Fe-N-P-Cl- doped carbon spheres with high-N-content of 16.85 % and ultrahigh specific surface area of 1434 m^2/g are prepared successfully and applied as electrocatalysts for ORR in alkaline media. The E_{onset} (1.14 V vs. RHE) and E_{half} (0.86 V vs. RHE) are both higher than 30% Pt/C benchmark catalyst,

confirming the good activity of the electrocatalyst. Based on the RRDE curves, the H_2O_2 yield is less that 2 % and the average electron transfer number is estimated to be 3.8, which is very close to 3.73−3.88 determined by RDE tests, slightly lower than that of 30% Pt/C (3.95). This suggests that the ORR catalysed by Fe-N-P-Cl- doped carbon spheres are carried out via an efficient four-electron pathway.

New approaches to the investigation of carbon formation in the Direct Synthesis of Methylchlorosilanes

Researcher: Dr. Mehdi Mahmoodinia
Project organization: Professor Hilde J. Venvik, Professor Edd A. Blekkan, Senior Scientist Torbjørn Røe (Elkem), Master students

This research is part of the innovation project (IPN), HECSI, between Elkem, NTNU, and SINTEF, aiming to design tailored silicon products and increase the productivity through improved understanding of chemistry of the Direct process or Müller-Rochow process:

$$CH_3Cl_{(g)} + Si_{(s)} \xrightarrow[300°C]{Cu-based_{(s)}} (CH_3)_xH_ySiCl_{z_{(g)}} \quad \text{where } x + y + z = 4$$

The dominant and main product of interest in this process is dimethyldichlorosilane, $(CH_3)_2SiCl_2$. However, this process faces several complications such as the carbon formation during the synthesis, which causes both economical and efficiency problems. The actual mechanism of the carbon formation, the nature of the carbon formed, and its relation to the process parameters remain to be understood to the extent that enables complete inhibition or a high degree of predictability. The main focus of this researcher project is to utilize the available analytical and characterization techniques and develop new methods for studying chloromethane cracking in order to establish correlations between materials and process parameters at the lab-scale.

Si/catalyst contact mass samples are prepared in Elkem's research laboratory at Fossegrenda, Trondheim, typically with a fluidized bed reactor, either in a batch or semi-continuous mode with gaseous reactant CH_3Cl feed, where the consumption of the solid reactant Si particles is compensated by periodic injections of fresh Si. The Cu based solid catalyst may also be compensated to some degree. Samples extracted from ongoing, as well as completed (stopped), fluidized bed experiments are transferred/stored through an inert routine and characterized under TGA/DSC/MS, Pyrolysis-GC/MS, Soxhlet extraction, FT-IR, Raman spectroscopy, XPS, XRD, AES, AFM and SEM/EDX. Methodology development for sample characterization is part of the work to further the understanding of the carbon deposition.

Financial support: The research is performed with financial support from the Research Council of Norway (Contract no. 295861) and Elkem Silicon Materials.

SINTEF projects

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

Steam and mixed reforming

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

The goal of this project is to support the client's efforts in developing catalysts for steam and mixed (steam + CO_2) reforming of methane at temperatures up to 950 °C and 30 bar. This involves testing of catalysts and analysis of gaseous products.
Client: BASF

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

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

Staff SINTEF (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

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

Fischer-Tropsch synthesis

Project category: Industry project

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

The objective of the project was evaluation of long time performance of a FT catalyst with different syngas compositions and how the catalyst is affected by syngas interruptions.

Client: VELOCYS

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 specifications incorporating biofuels 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 ASA

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

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

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

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

The main objectives of 4REFINERY are:

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

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

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

Publications:

Rune Lødeng, Håkon Bergem, Camilla Otterlei, Silje Fosse Håkonsen, Roman Tschentscher, *Catalytic co-hydroprocessing of rape seed and pyrolysis oil mixtures,* Poster presentation at 5th Int. Congress on Catalysis for Biorefineries (Catbior, 2019) 23-27 September, Turku, Finland.

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

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 (TelTek)

Staff SINTEF (WP4, co-HT and co-HDO, OMG lead): Senior Scientist Rune Lødeng, Research Scientist Håkon Bergem, Research Scientist Rune Myrstad and Senior Scientist Roman Tschentscher, Senior Scientist Anette Mathiesen

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 was 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 realis 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)

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

Staff (SINTEF): Senior Scientist Rune Lødeng

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

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

Publications:

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

Philosophiae Doctor (PhD) theses in 2019

Ata ul Rauf Salman - Friday, December 6
Catalysts for attaining NO / NO_2 equilibrium
Public trial lecture - Nitrogen fixation beyond Haber-Bosch - recent developments in heterogeneous catalysis and electrocatalysis

Martina Francisca Baidoo - Friday, April 26
Ethylene Oxychlorination on $CuCl_2$ based Catalysts: Operando Kinetic Study
Public trial lecture - Catalytic process for plastic recycling

Yalan Wang - Monday, March 4
Model-aided catalyst prediction through descriptor-based hybrid semi-empirical approach
Public trial lecture - Machine Learning in Heterogeneous Catalysis

Isaac Yeboah - Monday, February 25
Tandem Catalytic Upgrading of Biomass Fast-Pyrolysis Constituents to Fuels
Public trial lecture - Progress in single atom catalysis

Disputas Ata ul Rauf Salman, 6/12 2019. From left: Dr. Rune Lødeng, SINTEF, Dr Sang-Baek Shin fra Yara, Prof. Lars Pettersson, KTH, Ata ul Rauf Salman, Prof. Magnus Rønning, NTNU, Dr. David Waller, Yara, Prof. Hilde Venvik, NTNU.

Disputas Martina Francisca Baidoo, 26/4 2019. From left: Dr. Li He, NTNU, Prof. Enrico Tronconi, Politecnico di Milano, Italy, Prof. Unni Olsbye, UiO, Prof. De Chen. NTNU

Disputas Yalan Wang, 4/3 2018. From left: Prof. De Chen, NTNU, Dr. Kristofer Gunnar Paso, NTNU, Yalan Wang, Prof. Matteo Maestri, Politecnico, Milan, Italy, Prof. Stian Svelle, UiO.

Disputas Issac Yeboah, 25/2 2019. From left: Ass. Prof. II Kumar Ranjan Rout, SINTEF/NTNU, Prof. De Chen, NTNU, Prof. Yongdan Li, Alto University, Finland, Issac Yeboah, Prof. Magne Hillestad, NTNU, Rune Lødeng, SINTEF.

Master (Diploma) Students in 2019

Lisa Leganger Landfald: *Fe-ZSM-5 and Fe-SAPO-34 Catalysts for Low Temperature Selective Catalytic Reduction of NO_x by NH_3*

Minadir Saracevic: *NO to NO_2 oxidation over supported cobalt oxides catalysts*

Martin Meunche: *Advanced characterization of flame spray pyrolysis prepared catalysts for NO to NO_2 oxidation*

Kristiane Søvde Oftebro: *Synthesis and Characterization of Bismuth-containing Nanomaterials for Photocatalytic Ammonia Synthesis*

Erik Andreas Jørgensen: *Fischer-Tropsch Synthesis: Conversion of Bio-Syngas to Hydrocarbons*

Abdul Rahman Toutounji: *Methodology Development for the Characterization of Carbon Formed in the Direct Process*

Fatemeh Khodadady: *Process design and evaluation of CO_2 capture on solid sorbents*

Siyu Wang: *CO_2 capture at low temperature*

Tho Ba Tran: *One-pot catalytic vinyl chloride (VCM) production*

Dumitrita Spinu: *Bio Fuels from Lignin by Fast Pyrolysis with Coupled Catalytic Upgrading*

Exchange Master Students in 2019

Christian Maier: *Catalytic methane abatement of natural gas engines*

Asma Hayoune: *Photocatalytic H_2 production*

Henrik Schuster: *Catalytic Methane Abatement for Natural Gas Engines*

Constance Debonnie: *Polymers assisted preparation of Iron based Fischer-Tropsch Catalysts for biomass to fuel*

Group meetings 2019

KinCat
Catalysis Group – SINTEF – NTNU

Group meetings with seminars Catalysis Group, Spring 2019

Location: Room K5- 428/429

Schedule	Time	Presenter	Topic
January 25	14:00	Muhammad Zubair	Facile synthesis approach for core-shell TiO2–CdS nanoparticles for enhanced photocatalytic H2 generation from water.
February 8	14:00	Koteswara Rao Putta	Optimization of biomass entrained flow gasifier.
February 25		Issac Yeboah	Disputas
February 26	10:00	Yongdan Li (Gjesteforeleser)	Recent work on the anode of non-hydrogen solid oxide fuel cell.
March 4		Yalan Wang	Disputas
March 5	10:00	Matteo Maestri (Gjesteforeleser)	Structure-dependent microkinetic analysis of heterogeneous catalytic processes: methodology and applications.
March 15	14:00	Samuel K. Regli	Advanced in situ characterization of heterogeneous catalysts for sustainable process industry.
March 29			iCSI cleaning day.
April 5	14:00	Ainara Moral Larrasoana	Partial oxidation of methane with Co and Rh catalysts
April 26	10:00	Martina Francisca Baidoo	Disputas
May 10	14:00	Yanjing Qi	Prediction of barriers and adsorption energies in transition-metal heterogeneous catalysis by machine learning approaches.
May 24	14:00	Ljubisa Gavrilovic	Deactivation of the Cobalt Fischer-Tropsch Catalyst - a Kinetic Study
June 14	14:00	Li He	

KinCat
Catalysis Group – SINTEF – NTNU

Group meetings with seminars Catalysis Group, Fall 2019

Location: Room K5-428/429

Schedule	Time	Presenter	Topic
August 30	14:15	Xiaoli Yang	The conversion of syngas to aromatics via olefin routes. Combined microkinetic modeling and experimental study
September 6	14:15	Hilde Venvik	iCSI Midway evaluation – conclusion and outlook
September 20	13:15	Heinz J. Robota	Overview of Velocys technology
October 4	14:15	Stine Lervold	Morphology and activity of electrolytic silver catalyst for reactions relevant to partial oxidation of methanol to formaldehyde
October 18	14:15	Ingeborg-Helene Svenum	Sabbatical year in Madison
November 1	14:15	Hao Zhang	Structural evolution of Pt nanocluster under HER conditions.
November 15	14:15	Gang Wang	Surface tailoring of bifunctional Au-Ti catalyst for propylene epoxidation with H_2 and O_2.
November 29	14:15	Wenzhao Fu	Surface catalysis -mediated activity of hydrogen generation from ammonia borane on Ru-based catalysts.
December 6		Ata ul Rauf Salman	Disputas
December 2	0900	Tiejun Zhao	Mechanic strength: a key factor in industrial catalyst development
December 17			Julelunsj

Seminars/Guest lectures

Professor Yongdan Li, Alto University, Finland, will give a guest lecture:

Data: 10:00, Tuesday, February 26
Place: K5-429
Title: Recent work on the anode of non-hydrogen solid oxide fuel cell.

Professor Matteo Maestri, Department of Energy, Politecnico di Milano, Italy will give a guest lecture:

Data: 10:00, Tuesday, March 5
Place: K5-429
Title: Structure-dependent microkinetic analysis of heterogeneous catalytic processes: Methodology and applications.

Professor Enrico Tronconi, Department of Energy, Politecnico di Milano, Italy will give a guest lecture:

Data: 13:15, Thursday, April 25
Place: K5-429
Title: Fundamental and applied studies on NH_3-SCR over Cu-zeolites

Dr. Heinz J. Robota, Velocys will give a guest lecture (at the Group meeting):

Data: 13:15, Friday, September 20
Place: K5-429
Title: Overview of Velocys technology

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.

Learning methods and activities:

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 Industrial Chemistry and 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).

Learning methods and activities:

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

Course material:

J. Moulijn, M. Makkee and A. van Diepen: Chemical Process Technology

Wiley & Sons, 2nd edition, 2013, and articles and handouts.

Exam: Written

TKP4155 Reaction Kinetics and Catalysis

Responsible: Professor Magnus Rønning

Lecturers: Professor Magnus Rønning

Semester: Fall

Level: 4th year

Credits: 7.5 SP

Restricted Admission: No

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

Objectives:

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

Prerequisites:

Course TKP4110 Chemical Reaction Engineering or similar knowledge.

Contents:

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

Learning methods and activities:

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

Course material:

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

Exam: Written

TKP4190 - Fabrication and Applications of Nanomaterials

Responsible: Professor Jens-Petter Andreassen

Lecturers: Dr. Marie D. Strømsheim, 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 course starts by deriving the thermodynamic driving force and the kinetics of nucleation and growth of nanoparticles by 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. The classical crystallization theory is presented as the fundamental theoretical background and recently emerging alternative hypotheses are discussed.

Synthesis and functionalization of metallic and polymeric nanoparticles will be presented with an understanding of how growth can be controlled by tuning synthetic parameters. Functionalization of particle surfaces will be treated to tailor them towards specific applications. Solution based characterization techniques will be discussed from fundamental principles that are relevant for such nanomaterials.

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

Learning methods and activities:

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

The specialization involves the following courses:

TKP4580 - Catalysis and Petrochemistry, Specialization Project 15 SP

TKP4581 - Catalysis and Petrochemistry, Specialization Project 7.5 SP

TKP4515 - Catalysis, Specialization Course 7.5 SP

TKP4580/81 Catalysis and Petrochemistry, Specialization Project

Semester: Normally fall, adjustments in special cases

Level: 5th year.

Credits: 7.5 SP

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

Responsible: Engineer Karin W. Dragsten, Senior engineer Estelle Vanhaecke

Credits: The course is compulsory as a part of the specialization project.

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.

Learning methods and activities:
Seminars, demonstrations and instrument training.

Course material: Handouts

TKP4515 - Catalysis, Specialization Course

The course consists of 2 elective modules from the following list:

- Environmental catalysis - (3.75 SP).
- Heterogeneous catalysis (advanced course) - (3.75 SP).
- Industrial colloid chemistry - (3.75 SP).
- Reactor modelling - (3.75 SP).
- Chemical engineering, special topics - (3.75 SP).

Modules from other specializations can be chosen given the approval of the coordinator.

Semester: Fall

Level: 5th year.

Credits: 7.5 SP

Prerequisites: Industrial chemistry and refining and Kinetics and catalysis or similar courses.

Learning methods and activities: lectures, seminars, exercises, and self-study.

Course material: Handouts, Papers and Chapters from textbooks.

Language: English

Module 1 - Environmental and energy catalysis

Responsible: Professor Hilde J. Venvik

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 NO_X, sulfur etc., but also for the development of selective processes. The course will give the fundamentals for catalytic processes for purification of exhaust gases (NO_X, CO, unburned hydrocarbons etc.). Within energy production the focus is on biofuel production, catalytic combustion, production of H_2 and catalysis/reactor technology related to fuel cells. Catalysis for clean production is also included to the course. At the end of the course the students should be able to describe important applications of heterogeneous catalysts in energy conversion, emissions clean-up, and clean production.

Module 2 Heterogeneous catalysis, advanced course

Responsible: Professor Edd Anders Blekkan

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.

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 2019.

The course aims to give an understanding of the relation between modern theories of catalysis and the industrial application for the most important groups of heterogeneous catalysts; metals, metal oxides and zeolites. Assessment of the potential developments and limitations of catalysts will be analyzed through examples from industrial applications or processes under development. This includes the catalyst synthesis, a kinetic description of the different processes involved in a catalytic cycle (adsorption, surface reaction and desorption), mass and heat transfer issues, as well as interpretation of results from experimental and theoretical investigations.

Learning methods and activities: 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 2020.

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.

Learning methods and activities: Seminars.

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 2020

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 2019

1. **Buan, Marthe Emelie Melandsø; Cognigni, Andrea; Walmsley, John; Muthuswamy, Navaneethan; Rønning, Magnus.** Active sites for the oxygen reduction reaction in nitrogen-doped carbon nanofibers. *Catalysis Today* 2019 s.1-11

2. **Cao, Yueqiang; Fu, Wenzhao; Sui, Zhijun; Duan, Xuezhi; Chen, De; Zhou, Xinggui.** Kinetics Insights and Active Sites Discrimination of Pd-Catalyzed Selective Hydrogenation of Acetylene. *Industrial & Engineering Chemistry Research* 2019 ;Volum 58.(5) s.1888-1895

3. **Chang, Qing-Yu; Yin, Qiang; Ma, Fang; Zhu, Yi-An; Sui, Zhi-Jun; Zhou, Xing-Gui; Chen, De; Yuan, Wei-Kang.** Tuning Adsorption and Catalytic Properties of -Cr2O3 and ZnO in Propane Dehydrogenation by Creating Oxygen Vacancy and Doping Single Pt Atom: A Comparative First-Principles Study. *Industrial & Engineering Chemistry Research* 2019 ;Volum 58.(24) s.10199-10209

4. **Dam, Anh Hoang; Wang, Hongmin; Dehghan-Niri, Roya; Yu, Xiaofeng; Walmsley, John; Holmen, Anders; Yang, Jia; Chen, De.** Methane activation on bimetallic catalysts: properties and functions of surface Ni-Ag alloy. *ChemCatChem* 2019 ;Volum 11.(15) s.3401-3412

5. **Fu, Wenzhao; Chen, Wenyao; Qian, Gang; Chen, De; Yuan, Weikang; Zhou, Xinggui; Duan, Xuezhi.** Kinetics-assisted discrimination of active sites in Ru catalyzed hydrolytic dehydrogenation of ammonia borane. *Reaction Chemistry & Engineering* 2019 ;Volum 4.(2) s.316-322

6. **Gavrilovic, Ljubisa; Brandin, Jan; Holmen, Anders; Venvik, Hilde Johnsen; Myrstad, Rune; Blekkan, Edd Anders.** The effect of aerosol-deposited ash components on a cobalt-based Fischer–Tropsch catalyst. *Reaction Kinetics, Mechanisms and Catalysis* 2019;Volum 127.(1) s.231-240

7. **Gavrilovic, Ljubisa; Save, Jonas; Blekkan, Edd Anders.** The Effect of Potassium on Cobalt-Based Fischer– Tropsch Catalysts with Different Cobalt Particle Sizes. *Catalysts* 2019 ;Volum 9.(4)

8. **Hjorth, Ida; Nord, Magnus; Rønning, Magnus; Yang, Jia; Chen, De.** Electrochemical reduction of CO2 to synthesis gas on CNT supported CuxZn1-x O catalysts. *Catalysis Today* 2019 s.1-11

9. **Lervold, Stine; Arnesen, Kamilla; Beck, Nikolas; Lødeng, Rune; Yang, Jia; Bingen, Kristin; Skjelstad, Johan; Venvik, Hilde Johnsen.** Morphology and Activity of Electrolytic Silver Catalyst for Partial Oxidation of Methanol to Formaldehyde Under Different Exposures and Oxidation Reactions. *Topics in catalysis* 2019 ;Volum 62.(7-11) s.699-711

10. **Li, Yahao; Chen, Bingxu; Duan, Xuezhi; Chen, Shuangming; Liu, Daobin; Zang, Ketao; Si, Rui; Lou, Fengliu; Wang, Xuehang; Rønning, Magnus; Song, Li; Luo, Jun; Chen, De.** Atomically dispersed Fe-N-P-C complex electrocatalysts for superior oxygen reduction. *Applied Catalysis B: Environmental* 2019 ;Volum 249. s.306-315

11. **Weststrate, Kees-Jan; Mahmoodinia, Mehdi; Farstad, Mari Helene; Svenum, Ingeborg-Helene; Strømsheim, Marie Døvre; Niemantsverdriet, Hans; Venvik, Hilde Johnsen.** Interaction of hydrogen with flat (0001) and corrugated (11–20) and (10–12) cobalt surfaces: Insights from experiment and theory. *Catalysis Today* 2019 ;Volum 342. s.124-130

12. **Salman, Ata ul Rauf; Hyrve, Signe Marit; Regli, Samuel K.; Zubair, Muhammad; Enger, Bjørn Christian; Lødeng, Rune; Waller, David; Rønning, Magnus.** Catalytic Oxidation of NO

over LaCo1xBxO3 (B = Mn, Ni) Perovskites for Nitric Acid Production. *Catalysts* 2019 ;Volum 9.(5)

13. **Swirk, Katarzyna; Galvez, Maria Elena; Motak, Monika; Grzybek, Teresa; Rønning, Magnus; Da Costa, Patrick.** Syngas production from dry methane reforming over yttrium-promoted nickel-KIT-6 catalysts. *International journal of hydrogen energy* 2019 ;Volum 44.(1) s.274-286

14. **Swirk, Katarzyna; Rønning, Magnus; Motak, Monika; Beaunier, Patricia; Da Costa, Patrick; Grzybek, Teresa.** Ce- and Y-Modified Double-Layered Hydroxides as Catalysts for Dry Reforming of Methane: On the Effect of Yttrium Promotion. *Catalysts* 2019 ;Volum 9.(59) s.1-18

15. **Li, Qian; Yin, Qiang; Zheng, Ya-Shan; Sui, Zhi Jun; Zhou, Xinggui; Chen, De; Zhu, Yi-an.** Insights into Hydrogen Transport Behavior on Perovskite Surfaces: Transition from the Grotthuss Mechanism to the Vehicle Mechanism. *Langmuir* 2019 ;Volum 35.(30) s.9962-9969

16. **Li, Yahao; Chen, Bingxu; Duan, Xuezhi; Chen, Shuangming; Liu, Daobin; Zang, Ketao; Si, Rui; Lou, Fengliu; Wang, Xuehang; Rønning, Magnus; Song, Li; Luo, Jun; Chen, De.** Atomically dispersed Fe-N-P-C complex electrocatalysts for superior oxygen reduction. *Applied Catalysis B: Environmental* 2019 ;Volum 249. s.306-315

17. **Li, Yang; Cheng, W; Sui, Zhi jun; Zhou, Xinggui; Chen, De; Yuan, Wei-kang; Zhu, Yi-an.** Origin of Chemisorption Energy Scaling Relations over Perovskite Surfaces. *Journal of Physical Chemistry C* 2019 ;Volum 123.(46) s.28275-28283

18. **Li, Yang; Yang, Jie; Zhu, Yi-An; Sui, Zhi-Jun; Zhou, Xing-Gui; Chen, De; Yuan, Wei-Kang.** Surface phase diagrams of La-based perovskites towards the O-rich limit from first principles. *Physical Chemistry, Chemical Physics – PCCP* 2019 ;Volum 21.(24) s.12859-12871

19. **Li, Yang; Zheng, Ya-Shan; Zhu, Yi-An; Sui, Zhi-Jun; Zhou, Xing-Gui; Chen, De; Yuan, Wei-Kang.** BEEF-vdW+U method applied to perovskites: thermodynamic, structural, electronic, and magnetic properties. *Journal of Physics: Condensed Matter* 2019 ;Volum 31.(14) s.1-17

20. **Ma, Yuanyuan; Gan, Jie; Pan, Minjian; Zhang, Yanfang; Fu, Wenzhao; Duan, Xuezhi; Chen, Wenyao; Chen, De; Qian, Gang; Zhou, Xinggui.** Reaction mechanism and kinetics for Pt/CNTs catalyzed base-free oxidation of glycerol. *Chemical Engineering Science* 2019 ;Volum 203. s.228-236

21. **Noor, Tayyaba; Qi, Yanying; Chen, De.** Hydrogen dependence of the reaction mechanism and kinetics of water gas shift reaction on Ni catalyst: Experimental and DFT study. *Applied Catalysis B: Environmental* 2019 ;Volum 264.

22. **Qi, Yanying; Aaserud, Christian; Holmen, Anders; Yang, Jia; Chen, De.** Promotional effect of in-situ generated hydroxyl on olefin selectivity of Co-catalyzed Fischer-Tropsch synthesis. *Physical Chemistry, Chemical Physics - PCCP* 2019 ;Volum 21.(44) s.24441-24448

23. **Qi, Yanying; Yang, Jia; Holmen, Anders; Chen, De.** Investigation of C1+C1 Coupling Reactions in Cobalt-Catalyzed Fischer-Tropsch Synthesis by Combined DFT and Kinetic Isotope Study. *Catalysts* 2019 ;Volum 9.(6) s 551.

24. **Song, Zhaoning; Feng, Xiang; Sheng, Nan; Lin, Dong; Li, Yichuan; Liu, Yibin; Chen, Xiaobo; Chen, De; Zhou, Xinggui; Yang, Chaohe.** Cost-efficient core-shell TS-1/silicalite-1 supported Au

catalysts: Towards enhanced stability for propene epoxidation with H2 and O2. *Chemical Engineering Journal* 2019 ;Volum 377.

25. **Shafer, Wilson D.; Gnanamani, Muthu Kumaran; Graham, Uschi M; Yang, Jia; Masuku, Cornelius M; Jacobs, Gary; Davis, Burtron H..** Fischer-Tropsch: Product Selectivity-The Fingerprint of Synthetic Fuels. *Catalysts* 2019 ;Volum 9.(3) s.1-57

26. **Wang, Hai-Zhi; Zhang, Wei; Jiang, Jia-Wei; Sui, Zhi-Jun; Zhu, Yi-An; Ye, Guang-Hua; Chen, De; Zhou, Xing-Gui; Yuan, Wei-Kang.** The role of H2S addition on Pt/Al2O3 catalyzed propane dehydrogenation: a mechanistic study. *Catalysis science & technology* 2019 ;Volum9.(3) s.867-876

27. **Wang, Yalan; Wang, Hongmin; Dam, Anh Hoang; Xiao, Ling; Qi, Yanying; Niu, Juntian; Yang, Jia; Zhu, Yi-An; Holmen, Anders; Chen, De.** Understanding effects of Ni particle size on steam methane reforming activity by combined experimental and theoretical analysis. *Catalysis Today* 2019 s.1-9

28. **Wang, Yalan; Xiao, Ling; Qi, Yanying; Mahmoodinia, Mehdi; Feng, Xiang; Yang, Jia; Zhu, Yi-An; Chen, De.** Towards rational catalyst design: boosting the rapid prediction of transition-metal activity by improved scaling relations. *Physical Chemistry, Chemical Physics - PCCP* 2019 ;Volum 21.(35) s.19269-19280

29. **Yin, Qiang; Ma, Fang; Zhou, Yan; Sui, Zhi-Jun; Zhou, Xing-Gui; Chen, De; Zhu, Yi-An.** Size-Dependent Segregation Preference in Single-Atom Alloys of Late Transition Metals: Effects of Magnetism, Electron Correlation, and Geometrical Strain. *Journal of Physical Chemistry C* 2019 ;Volum 123.(30) s.18417-18424

30. **Zhang, Zhihua; Zhao, Xuan; Wang, Gang; Xu, Jialun; Lu, Mengke; Fu, Wenzhao; Duan, Xuezhi; Qian, Gang; Chen, De; Zhou, Xinggui.** Uncalcined TS2 immobilized Au nanoparticles as a bifunctional catalyst to boost direct propylene epoxidation with H2 and O2. *AIChE Journal* 2019 ;Volum 66.(2)

31. **Zheng, Ya-Shan; Zhang, Min; Li, Qian; Zhu, Yi-An; Sui, Zhi-Jun; Chen, De; Zhou, Xing-Gui.** Electronic Origin of Oxygen Transport Behavior in La-Based Perovskites: A Density Functional Theory Study. *Journal of Physical Chemistry C* 2019 ;Volum 123.(1) s.275-290

32. **Zhou, Haitao; Liu, Chao; Wu, Jian-Chun; Liu, Menghao; Zhang, Dong; Song, Honglei; Zhang, Xiaoyun; Gao, Hongquan; Yang, Jianhong; Chen, De.** Boosting the electrochemical performance through proton transfer for the Zn-ion hybrid supercapacitor with both ionic liquid and organic electrolytes. *Journal of Materials Chemistry A* 2019 ;Volum 7.(16) s.9708-9715

33. **Zhu, Xiaojuan; Qishui, Guo; Sun, Yafei; Chen, Shangjun; Wang, Jian-Qiang; Wu, Mengmeng; Fu, Wenzhao; Tang, Yanqiang; Duan, Xuezhi; Chen, De; Wan, Ying.** Optimising surface d charge of AuPd nanoalloy catalysts for enhanced catalytic activity. *Nature Communications* 2019 ;Volum 10.(1428) s.1-11

34. **Zhou, Haitao; Liu, Chao; Wu, Jian-Chun; Liu, Menghao; Zhang, Dong; Song, Honglei; Zhang, Xiaoyun; Gao, Hongquan; Yang, Jianhong; Chen, De.** Boosting the electrochemical performance through proton transfer for the Zn-ion hybrid supercapacitor with both ionic liquid and organic electrolytes. *Journal of Materials Chemistry A* 2019 ;Volum 7.(16) s.9708-9715

35. **Rytter, Borg, Øyvind; Enger, Bjørn Christian; Holmen, Anders.** α-alumins as catalyst support in Co Fischer-Tropsch synthesis and the effect of added water; encompassing transienr effects. *J. Catal. 2019; Volum 373 s 13-24.*

Presentations in 2019

1. **Bjørkedal, Ole Håvik; Regli, Samuel K.; Rønning, Magnus.** Cu-containing mesoporous alumina as catalysts for SCR. EuropaCat 2019; 2019-08-18 - 2019-08-23

2. **Cai, Zhenping; Feng, Xiang; Chen, De.** co-pyrolysis of biomass and polyethylene into C2-C4 olefins over zeolite catalyst. The 11th International Conference on Applied Energy (ICAE2019); 2019-08-12 - 2019-08-15

3. **Casalegno, Mario Ernesto; Tsakoumis, Nikolaos; Rout, Kumar Ranjan; Blekkan, Edd Anders; Chen, De.** Aspen Plus simulations of Steam Ethanol Reforming and promoted Co-Ni/Hydrotalcite structures: Process and catalyst optimization. The Norwegian Catalysis Symposium 2019; 2019-12-05 - 2019-12-06

4. **Cazzolaro, Martina; Yang, Jia; Svendby, Jørgen; De Clercq, Rik; Beier, Matthias Josef; Taarning, Esben; Chen, De.** Stable Cu/C catalysts for selective hydrogenation of hydroxyacetone to propylene glycol. Building a sustainable European biofuel industry; 2019-11-04 - 2019-11-06

5. **Cazzolaro, Martina; Yang, Jia; Svendby, Jørgen; De Clercq, Rik; Beier, Matthias Josef; Taarning, Esben; Chen, De.** Stable Cu/C catalysts for selective hydrogenation of hydroxyacetone to 1,2-propanediol. 14th European Congress on Catalysis, EuropaCat 2019; 2019-08-18 - 2019-08-23

6. **Chen, Qingjun; Rout, Kumar Ranjan; Wang, Siyu; Chen, De.** PEI Impregnated Mesoporous Carbon Spheres As Ideal Sorbent for Post-Combustion CO2 Capture from Natural Gas Power Plant. 12th Natural gas conversion symposium; 2019-06-02 - 2019-06-08

7. **Chen, Qingjun; Wang, Siyu; Rout, Kumar Ranjan; Chen, De.** Development of Polyethylenimine (PEI)-Impregnated Mesoporous Carbon Spheres for low-concentration CO2 Capture from Natural Gas PowerPlant. CLIMIT phD and postdoc seminar; 2019-01-18 - 2019-01-19

8. **Gavrilovic, Ljubisa; Brandin, Jan; Holmen, Anders; Venvik, Hilde Johnsen; Myrstad, Rune; Rout, Kumar Ranjan; Rytter, Erling; Hillestad, Magne; Blekkan, Edd Anders.** Deactivation of the Cobalt Fischer-Tropsch catalyst – a Kinetic Study. 12th Natural Gas Conversion Symposium; 2019-06-02 - 2019-06-06

9. **Gavrilovic, Ljubisa; Runningen, Anders; Jørgensen, Erik Andreas; Pandey, Umesh; Putta, Koteswara Rao; Rout, Kumar Ranjan; Rytter, Erling; Hillestad, Magne; Blekkan, Edd Anders.** Modeling Fischer-Tropsch kinetics for reactor design. Building a sustainable European biofuel industry; 2019-11-04 - 2019-11-06

10. **Gavrilovic, Ljubisa; Runningen, Anders; Jørgensen, Erik Andreas; Pandey, Umesh; Putta, Koteswara Rao; Rout, Kumar Ranjan; Rytter, Erling; Hillestad, Magne; Blekkan, Edd Anders.** Modeling Fischer-Tropsch kinetics for reactor design. 26th meeting of the North American Catalysis Society, NAM26; 2019-06-23 - 2019-06-28

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13. **Lervold, Stine; Arnesen, Kamilla; Beck, Nikolas; Lødeng, Rune; Yang, Jia; Bingen, Kristin; Skjelstad, Johan; Venvik, Hilde Johnsen.** Morphology and activity of electrolytic silver catalyst - For reactions relevant to partial oxidation of methanol to formaldehyde (MTF). EuropaCat 2019; 2019-08-18 - 2019-08-23

14. **Ma, Jianyu; Rout, Kumar Ranjan; Sauer, Maximilian; Mahmoodinia, Mehdi; Blekkan, Edd Anders.** INVESTIGATIONS OF MOLYBDENUM-PROMOTED MANGANESE-BASED SOLID SORBENTS FOR H2S CAPTURE. 17th International Conference on Clean Energy (ICCE-2019); 2019-08-09 - 2019-08-12

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17. **Mahmoodinia, Mehdi; Ma, Jianyu; Sauer, Maximilian; Rout, Kumar Ranjan; Blekkan, Edd Anders.** Performance of Manganese-based Solid Sorbents for H2S Removal: Particle Size and Promoter Effects on Sorbent Capacity. Geet19-Green Energy and Environmental Technology; 2019-07-24 - 2019-07-26

18. **Pandey, Umesh; Putta, Koteswara Rao; Gavrilovic, Ljubisa; Rout, Kumar Ranjan; Rytter, Erling; Blekkan, Edd Anders; Hillestad, Magne.** Optimization of advanced biofuel production via Fischer-Tropsch synthesis. Building a sustainable European biofuel industry; 2019-11-04 - 2019-11-06

19. **Pedersen, Eirik Østbye; Svenum, Ingeborg-Helene; Blekkan, Edd Anders.** Mn-promoted cobalt catalysts for light olefin production. ACS Spring 2019 National Meeting & Exposition; 2019-03-31 - 2019-04-02

20. **Putta, Koteswara Rao; Rout, Kumar Ranjan; Rytter, Erling; Blekkan, Edd Anders; Hillestad, Magne.** Kinetic modelling and validation of entrained flow biomass gasifier for syngas production for FT-synthesis. Building a sustainable European biofuel industry; 2019-11-04 - 2019-11-06

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22. **Rønning, Magnus.** Characterisation of Fischer-Tropsch synthesis catalysts at industrial working conditions. DynaCat Kick-off Meeting SPP 2080; 2019-02-11 - 2019-02-12

23. **Rønning, Magnus.** Combination of operando characterisation techniques for studies of catalysts at work. Operando Surface Catalysis meeting (OPSCAT); 2019-01-29 - 2019-02-01

24. **Salman, Ata ul Rauf; Regli, Samuel K.; Enger, Bjørn Christian; Lødeng, Rune; Waller, David; Rønning, Magnus.** Revealing the Structural and Chemical State of Platinum Nanoparticles during Oxidation of NO to NO2 at Nitric Acid Plant Conditions. 2019 North American Catalysis Society Meeting; 2019-06-23 - 2019-06-28

25. **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. Operando Surface Catalysis meeting; 2019-01-29 - 2019-02-01

26. **Strømsheim, Marie Døvre; Svenum, Ingeborg-Helene; Mahmoodinia, Mehdi; Boix, Virginia; Knudsen, Jan; Venvik, Hilde Johnsen.** Investigations of the surface dynamics of Pd-alloy surfaces under oxidation reactions. 6th annual APXPS Workshop; 2019-12-10 - 2019-12-13

27. **Sunding, Martin Fleissner; Jensen, Ingvild Julie Thue; Svenum, Ingeborg-Helene; Ivashenko, Oleksii; Redekop, Evgeniy; Wells, Justin; Fagerberg, Ragnar; Sjåstad, Anja Olafsen; Venvik, Hilde Johnsen; Olsbye, Unni; Diplas, Spyridon.** National Surface and Interface Analysis Laboratory (NICE II): From (near) in-situ to operando XPS analysis. OPSCAT; 2019-01-29 - 2019-02-01

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29. **Svenum, Ingeborg-Helene; Vicinanza, Nicla; Herron, Jeffrey A.; Mavrikakis, Manos; Venvik, Hilde Johnsen.** Effects of Surface Phenomena on the Performance of Pd-Ag Membranes. Group meeting at UW-Madison; 2019-02-10

30. **Tafjord, Joakim; Nerb, Johannes; Myrstad, Rune; Blekkan, Edd Anders; Holmen, Anders; Yang, Jia.** Effect of Potassium on Highly Dispersed Fe-Nanoparticles Supported on Carbon for CO hydrogenation. 12th Natural Gas Conversion Symposium; 2019-06-02 - 2019-06-06

31. **Tomasgard, Asgeir; Berstad, David Olsson; Burheim, Odne Stokke; Blekkan, Edd Anders; Dawson, James; Espegren, Kari Aamodt; Karstad, Per Ivar; Løvås, Terese; Meyer, Julien; Møller-Holst, Steffen; Nekså, Petter; Pollet, Bruno G.; Størset, Sigmund Østtveit; Sundseth, Kyrre; Thomassen, Magnus; Ulleberg, Øystein.** Hydrogen i fremtidens lavkarbonsamfunn. Trondheim: Center for Sustainable Energy Research (CenSES), NTNU 2019 (ISBN 978-82-93198-31-4) 40 s.

32. **Tsakoumis, Nikolaos; Casalegno, Mario Ernesto; Wang, Yalan; Blekkan, Edd Anders; Chen, De.** Extra pure hydrogen production for mobile applications An integrated approach. NTNU Team Hydrogen Annual Workshop; 2019-12-02 - 2019-12-03

33. **Tsakoumis, Nikolaos; Casalegno, Mario Ernesto; Wang, Yalan; Rout, Kumar Ranjan; Blekkan, Edd Anders; Chen, De.** Steam Ethanol Reforming on Promoted Co-Ni/Hydrotalcite Structures: Catalyst Optimization. 2019 North American Catalysis Society Meeting; 2019-06-23 - 2019-06-28

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of H2-CO-H2 Activation Treatment. 2019 North American Catalysis Society Meeting; 2019-06 23 - 2019-06-28

35. **Venvik, Hilde Johnsen.** iCSI – industrial Catalysis Science and Innovation for a competitive and sustainable process industry. Operando Surface Catalysis meeting (OPSCAT); 2019-01-29 - 2019-02-01

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37. **Feng, Xiang; Cai, Zhenping; Chen, De.** Enhanced aromatics generation from catalytic pyrolysis of woody biomass over hollow structured HZSM-5 catalyst. The 11th International Conference on Applied Energy (ICAE2019); 2019-08-12 - 2019-08-15

38. **Guo, Xiaoyang; Vanhaecke, Estelle Marie M.; Vullum, Per Erik; Ma, Jianyu; Gunawardana, Daham; Walmsley, John; Chen, De; Venvik, Hilde Johnsen.** The initial stage of Metal Dusting Corrosion of Inconel 601 – effects of exposure conditions and near-surface structure and composition. 12th Natural Gas Conversion Symposium - NGCS12; 2019-06-02 - 2019-06-06

39. **Liland, Shirley Elisabeth Sjø; Rout, Kumar Ranjan; Chen, De.** Understanding the redox reactions of Ni and Co during catalytic combustion of methane. The 12th Natural Gas Conversion Symposium; 2019-06- 02 - 2019-06-06

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41. **Ma, Hongfei; Fenes, Endre; Qi, Yanying; Rout, Kumar Ranjan; Fuglerud, Terje; Chen, De.** Alkali Metal Doping of Ethylene Oxychlorination Catalysts: Chemistry, Kinetics and Descriptors. 14th European Congress on Catalysis; 2019-08- 18 - 2019-08-23

42. **Ma, Hongfei; Fenes, Endre; Qi, Yanying; Rout, Kumar Ranjan; Fuglerud, Terje; Chen, De.** Kinetic Analysis and Design of Catalytic Redox Cycles. NAM26, 2019 North American Catalysis Society Meeting; 2019-06-23 - 2019-06-26

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44. **Pan, Minjian; Wang, Jingnan; Fu, Wenzhao; Chen, Bingxu; Lei, Jiaqi; Chen, Wenyao; Duan, Xuezhi; Chen, De; Qian, Gang; Zhou,Xinggui.** Active sites of Pt/CNTs nanocatalysts for aerobic base-free oxidation of glycerol. *Green Energy & Environment* 2019 s.1-7

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46. **Qian, Weixin; Wang, Yalan; Yang, Jia; Chen, De.** Rational design of Cu based bimetallic catalysts for higher alcohols synthesis by combined micro-kinetic modeling and experiments. 14th European Congress on Catalysis, EuropaCat 2019; 2019-08-18 - 2019-08-23

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50. **Rout, Kumar Ranjan; Gil Matellanes, Maria Victoria; Chen, De.** Highly selective CO removal by sorption enhanced Boudouard reaction for hydrogen production. *Catalysis science & technology* 2019 ;Volum 9.(15) s.4100-4107

51. **Rout, Kumar Ranjan; Yeboah, Isaac; Feng, Xiang; Chen, De.** Tandem Catalytic Reactions System for Upgrading of Bio-vapors of Fast-hydropyrolysis of Biomass to Biofuels,. North American Catalysis Society Meeting; 2019-06-23 - 2019-06-28

52. **Selleri, Tommaso; Hu, Wenshuo; Gramigni, Federica; Fenes, Endre; Ma, Hongfei; Rout, Kumar Ranjan; Nova, Isabella; Tronconi, Enrico; Chen, De.** Study of the reduction half-cycle in the low temperature Selective Catalytic Reduction of NO over Cu-SSZ-13. 14th European Congress on Catalysis; 2019-08-18 - 2019-08-23

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54. **Skodvin, Daniel; Chen, De.** Carbon Nanomaterial-IL Hybrids for Ultrahigh Energy Supercapacitors. European Materials Research Society; 2019-03-27 - 2019-03-31

55. **Spinu, Dumitrita; Chen, De; Rout, Kumar Ranjan.** Lignin to Bio-fuels via Fast Pyrolysis Process Assisted by Volatiles Catalytic Upgrading. Building a sustainable European biofuel industry; 2019-11-04 - 2019-11-06

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65. **Cazzolaro, Martina; Yang, Jia; Svendby, Jørgen; De Clercq, Rik; Beier, Matthias Josef; Taarning, Esben; Chen, De.** Stable Cu/C catalysts for selective hydrogenation of hydroxyacetone to propylene glycol. Building a sustainable European biofuel industry; 2019-11-04 - 2019-11-06

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67. **Lervold, Stine; Arnesen, Kamilla; Beck, Nikolas; Lødeng, Rune; Yang, Jia; Bingen, Kristin; Skjelstad, Johan; Venvik, Hilde Johnsen.** Morphology and activity of electrolytic silver catalyst - For reactions relevant to partial oxidation of methanol to formaldehyde (MTF). EuropaCat 2019; 2019-08-18 - 2019-08-23

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74. **Zubair, Muhammad; Rønning, Magnus; Yang, Jia.** Artificial photosynthesis for H2 generation from water employing CdS@TiO2 nanostructures. Spring meeting: Norwegian Academy of Technological Sciences; 2019-03-28 - 2019-03-28

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_2-C_4) alkanes by catalytic processes*. 1995

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

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

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

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

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

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

Magnus Rønning: *Photocatalysis*. 2/3 2000

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

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

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

Lucie Bednarova: *Computational Catalysis*. 2002

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

Leiv Låte: *Catalysis in supercritical fluids*. 2002

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

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

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

Kjetil Hauge: *Non-conventional routes to petrochemicals and fuels 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

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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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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Martina Francisca Baidoo: *Catalytic process for plastic recycling.* 26/4 2019

Yalan Wang: *Machine Learning in Heterogeneous Catalysis* 4/3 2019

Isaac Yeboah: *Progress in single atom catalysis 25/2 2019*

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
Diffusjon 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/Al2O3 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 C4–C6 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: Kuiper & Burger Advies- en Ingenieursbureau, 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_2 catalysts supported on carbon nanostructures for CO removal reactions
Defense of thesis: November 2008
Current position: Yara, Porsgrunn.

Astrid Lervik Mejdell
Properties and application of 1-5µm 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_2 Acceptors for Sorption Enhanced Steam Methane Reforming
Defense of thesis: November 2011.

Navaneethan Muthuswamy
Platinum based Catalysts for Methanol Fuel Cells: Metal Clusters and Carbon Supports.
Defense of thesis: December 2011
Current positions: Researcher, NTNU.

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

Eleni Patanou
Adsorption Microcalorimetry studies on Cobalt Catalysts
Defense of thesis: September 2012
Current position: 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: Beyonder AS, Stavanger.

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

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

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

Georg Voss
Mesostructured alumina and the state of Ni as promotor for Co Fischer-Tropsch synthesis catalysts.
Defense of thesis: August 2014
Current position: 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 CO2 in aqueous solutions
Defense of thesis: March 31 2017
Current position: NAMMO, Raufoss.

Marie Døvre Strømsheim
Co{11-20} and Pd3Au{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: FFI

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.

Isaac Yeboah
Tandem Catalytic Upgrading of Biomass Fast-Pyrolysis Constituents to Fuels
Defense of thesis: February 25, 2019
Current position: Ineos, USA.

Yalan Wang
Model-aided catalyst prediction through descriptor-based hybrid semi-empirical approach
Defense of thesis: March 4, 2019
Current position: Post.Doc. NTNU.

Martina Francisca Baidoo
Ethylene Oxychlorination on $CuCl_2$based Catalysts: Operando Kinetic Study.
Defense of thesis: April 26, 2019
Current position: Kwame Nkrumah University of Science and Technology, Ghana.

Ata ul Rauf Salman
Catalysts for attaining NO/NO_2 equilibrium
Defense of thesis: December 6, 2019
Current position: Equinor