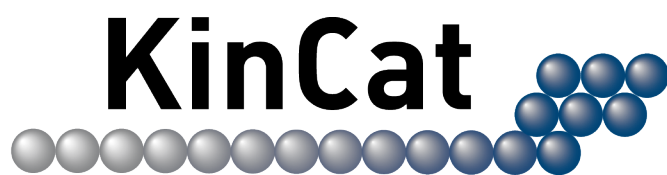


Annual Report

2021



Catalysis Group – SINTEF – NTNU

Gemini Centre

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 collaboration between their members. It consists of the Catalysis Group, Department of Chemical Engineering, NTNU and the catalysis research team, SINTEF Industry. As of January 2008, the KinCat has been established as a Gemini Centre by NTNU and SINTEF.

KinCat addresses:

Department of Chemical Engineering, NTNU
Catalysis group
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>

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Annual Report 2021
KinCat
Strong Point Centre Kinetics and Catalysis

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Members of KinCat

Catalysis Group, Department of Chemical Engineering, NTNU

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
Adjunct Assoc. Prof. David Waller

SFI-coordinator

Dr. Anne Hoff (60%)

Technical Staff

Engineer Karin Wiggen Dragsten (until September 2021)
Senior Engineer Dr. Estelle Marie M. Vanhaecke
Senior Engineer Samuel K. Regli (since October 2021)
Senior Engineer Dr. Anne Hoff (10%)

Doctoral candidates 2021

Ole H. Bjørkedal
Björn Frederik Baumgarten
Samuel K. Regli
Daniel Skodvin
Martina Cazzolaro
Mario Ernesto Casalegno
Joakim Tafjord
Jibin Antony
Moses Mawanga
Ask Lysne
Dumitrita Spinu
Junbo Yu
Monica Pazos Urrea

Petter Tingelstad
Youri van Valen
Oscar Luis Ivanez Encinas
Jithin Gopakumar
Kishore Rajendran
Wei Zhang
Zhihui “Zoe” Li
Albert Miró i Rovira
Stine Lervold (defended 2021)
Hongfei Ma (defended 2021)
Muhammad Zubair (defended 2021)
Endre Fenes (defended 2021)
Jianyu Ma (defended 2021)

Postdoctoral fellows/Researchers

Dr. Hongfei Ma
Dr. Xiaoyang Guo
Dr. Felix Herold
Dr. Ainara Moral Larrasoana
Dr. Marie Døvre Strømsheim

Dr. Mehdi Mahmoodinia
Dr. Yalan Wang
Dr. Tina Bergh
Dr. Balasingam Suresh Kannan
Dr. Katarzyna Swirk

Visitors 2021

Aldo Lanza
Yurou Li

Dong Lin
Consolato Rosmini

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

Gunn Torill Wikdahl (HSE)
Merete Christensen (purchaser)
Ketil Torset Helland (workshop)

Erland Strendo (workshop)
Mikael Hammer (electrical support)
Christopher Sørmo (purchaser, waste)

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
Res. Scientist Nikolaos Tsakoumis

Master of Science Shirley Liland
Senior Scientist Kumar R. Rout
Research Scientist Rune Myrstad
Senior Scientist Rune Lødeng

Laboratory personnel

Senior Engineer Camilla Otterlei

Group Members



Edd A. Blekkan



De Chen



Magnus Rønning



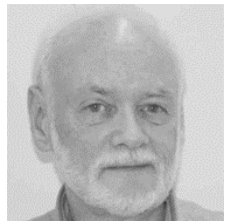
Hilde J. Venvik



Jia Yang



Anders Holmen



Erling Rytter



Kjell Moljord



Ingeborg-Helene
Svenum



Kumar R. Rout



David Waller



Anne Hoff



Estelle Marie M.
Vanhaecke



Samuel K. Regli



Karin W. Dragsten



Ole H. Bjørkedal



Björn F.
Baumgarten



Daniel Skodvin



Martina Cazzolaro



Mario Ernesto
Casalegno



Joakim Tafjord



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Moses Mawanga



Ask Lysne



Dumitrita Spinu



Junbo Yu



Monica Pazos
Urrea



Petter Tingelstad



Youri van Valen



Oscar Luis Ivanez
Encinas



Jithin Gopakumar



Kishore Rajendran



Wei Zhang



Zihui «Zoe» Li



Albert Miró i
Rovira



Yurou Li



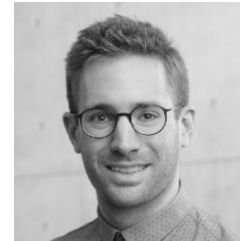
Tina Bergh



Mehdi
Mahmoodinia



Xiaoyang Guo



Felix Herold



Muhammad Zubair



Endre Fenes



Hongfei Ma



Jianyu Ma



Stine Lervold



Marie Døvre
Strømsheim



Ainara Moral
Larrasoana



Yalan Wang



Suresh Kannan
Balasingam



Katarzyna Swirk



Torbjørn Gjervan



Kirsti Blomsøy



Håkon Bergem



Bjørn Christian
Enger



Rune Lødeng



Rune Myrstad



Nikolaos E.
Tsakoumis



Shirley E. Liland



Kumar R. Rout



Camilla Otterlei

Research Areas

Conversion of natural gas

- Synthesis gas and hydrogen production
- Fischer-Tropsch synthesis
- Dehydrogenation of ethane and propane
- Solid acceptors for CO₂-capture
- Production of methanol and dimethyl ether (DME)
- Direct methane conversion

Industrial catalysis

- Oxychlorination
- Catalytic oxidation of NO to NO₂
- Catalytic oxidation of methanol to formaldehyde
- Methylchlorosilanes

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
- CO₂ reduction

-
- 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 H₂S removal.
- Sorbents and processes for CO₂ capture
- Pd based hydrogen separation membranes

Photocatalysis

- Water splitting
- Photo reforming
- Nitrogen fixation

Material integrity

- Metal dusting corrosion

Main Laboratory Equipment

Reaction laboratories

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

Catalyst preparation laboratory

- Glove box for electrochemistry
- Chemical Vapor Deposition (CVD) setups for carbon synthesis
- Stirred pressure reactors/autoclaves
- Centrifuge
- CVD
- Milling machine
- Vacuum oven
- Rotary evaporator
- Spray dryer
- Ball mills
- Granulation equipment
- Calcination set-up

Catalyst characterization

- Catalyst characterization equipment with CO chemisorption, Temperature Programmed Reduction/Oxidation/Desorption capabilities
- Chromatography of product streams by GC, GC-MS or HPLC-MS
- Thermogravimetric analysis (TGA)

-
- Differential scanning calorimetry (DSC)
 - Chemisorption (CO, H₂ or CO₂)
 - Surface area and porosity analysis by nitrogen adsorption (BET)
 - Wavelength Dispersive X-ray Fluorescence for powders and liquids from O through U
 - Scanning tunneling microscope (STM)
 - Potentiostat for battery/electrochemical cell studies
 - X-ray fluorescence (XRF)

Advanced *in situ* and *operando* characterization

- LabXxS (in-house XAFS and XES, currently only *ex situ*)
- Raman (325, 633 and 785 nm)
- DRIFTS (MidIR)
- Diffuse reflectance UV-vis probes

Instrumentation in regular use in other NTNU departments

- Transmission Electron Microscopy (TEM) and related techniques @NORTEM, NTNU
- X-ray photoelectron spectroscopy (XPS), Scanning transmission electron microscopy (STEM), Focused ion beam (FIB) sputtering and various synthesis, structuring, and sample treatment facilities @NTNU Nanolab
- X-ray diffraction (XRD) and Scanning electron microscopy (SEM) @Department of Materials Science and Engineering, NTNU

Instrumentation accessed at international facilities and/or in international collaboration

- Synchrotron X-ray diffraction (XRD) and absorption (XANES, EXAFS) at the Swiss-Norwegian Beamlines (SNBL) of the European Synchrotron Radiation Facility (ESRF)
- High resolution X-ray photoelectron spectroscopy (XPS) and Near-ambient pressure X-ray photoelectron spectroscopy (APPES) at the MAX IV Synchrotron Laboratory

Highlights from Activities in 2021

- ❖ The Corona pandemic has had a great impact on the activity also in 2021, on teaching as well as on laboratory work. Group meetings, seminars, etc. have all been digital. As a consequence of travel restrictions, very few attended international meetings.
- ❖ Five candidates completed their PhD degree in 2021: Jianyu Ma, Endre Fenes, Muhammad Zubair, Hongfei Ma and Stine Lervold. The title of the dissertation, the title of the trial lecture and pictures of the candidate/committees/supervisors are enclosed.
- ❖ 10 M.Sc. students completed their thesis in 2021. Their names and titles of the thesis are enclosed. 2 exchange students also completed their thesis.
- ❖ 59 publications in International Journals including papers in prestigious journals: Angewandte Chemie International Edition (De Chen, Kumar Rout et al.) and Nature Communications (De Chen et al).
- ❖ 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 NTNU, UiO and SINTEF as the academic partners. NTNU is the Centre host with Professor Hilde J. 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 CATHEX project with support from the Research Council of Norway is a large network running to 2025. Due to the pandemic, it was only possible to organize webinars in 2021. A description of the project is enclosed.
- ❖ The 2021 iCSI Annual Seminar took place October 18-19 at Hovde gård, across the fjord from Trondheim. The program is enclosed.
- ❖ The group organized a KinCat seminar during September 16-17 at Bortistu Gjestegård. The program is enclosed.
- ❖ A laboratory X-ray absorption – X-ray emission spectrometer has been installed in our laboratories.
- ❖ A collaboration platform between Quantafuel and the Department of Chemical Engineering is established. The Innovation hub was officially opened on 11th October 21. The program of the opening is enclosed.
- ❖ The catalysis group runs a bi-weekly seminar. The programs are enclosed.

-
- ❖ The group is a research partner in BIO4FUELS, a Centre for Environment - friendly Energy Research (FME), hosted by The Norwegian University of Life Sciences (NMBU). The Center has a total budget of around 270 MNOK over 8 years and covers all important value-chains for conversion of lignocellulosic biomass to biofuels. User partners are key national and international industries, as well as forestry owners and regional authorities. Our activities are related to catalytic processes for 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, H₂MemX, Swiss-Norwegian Beamlines, UK Catalysis Hub, Eurokin, NanoCat4Fuels and KPN Biomass to aviation fuels (B2A).
 - ❖ The group participates in several EU-projects and networks: MSCA Innovative Training Network (BIKE), MSCA Individual Fellowship (Meso-SiO₂), MSCA-Rise (OPYIMA). Research and Innovation action: (EHL CATHOL).
 - ❖ Strategic support from NTNU consisting of PhD fellowship grants and financial support.

**industrial Catalysis Science and Innovation
for a competitive and sustainable process industry**



Summary Activity 2021

- ❖ Although 2021 started off in a similar manner to what had been the case through most of 2020, iCSI work was able to proceed almost normally with open laboratories all year. The vaccination program gave a boost to the hope of better times. However, travel restrictions and quarantine requirements made international cooperation difficult, and beam times in European laboratories in particular had to be cancelled or postponed.
- ❖ Educating master students is important to iCSI. In 2021, eleven graduating master students were associated with iCSI, of whom two delivered directly into the ongoing projects. The gender balance within iCSI is maintained, with all personnel categories within a 40/60 distribution.
- ❖ In 2021, iCSI finalized the centre's employment plan by welcoming the three final candidates: Postdoctoral fellow Tina Bergh and PhD candidate Björn Frederik Baumgarten at NTNU, and PhD candidate Bjørn Gading Solemsli at UiO (being respectively the 6th postdoc and the 14th and 15th PhDs within iCSI). Three candidates (Endre Fenes, Hongfei Ma and Stine Lervold) finalized their PhD theses with two defences in March and one in June, respectively. iCSI congratulates them!
- ❖ The high publishing activity has continued from last year, and 23 reviewed papers were accepted and published in 2021. As in the previous year, Innovation Area 4 (PVC Value Chain: World Class Energy and Raw Material Efficiency for the Production of Chlorine and Vinyl Chloride Monomer) kept going with a high publication rate, but also IIA1, 3, 5 and 6 have published several papers.
- ❖ Once more, lack of travel and conference participation are reflected in the list of conference contributions. Most of the presentations are from the iCSI Annual Seminar, which after two postponements, fortunately could take place at Hovde gård in October. A few international *digital* events took place, however, and some of them had invited lecturers from iCSI.

-
- ❖ The science is progressing in all Industrial Innovation Areas (IIAs), and this is exemplified by an annual highlight: A goal in IIA1 has been to explain why the Pd/Ni net used in the production of nitric acid for fertilizers, transforms into something similar to a porous plate during industrial operation. This change results in a significant pressure drop through the gauze pack, limiting the number of Pd/Ni gauzes which can be installed simultaneously. The answer revealed by Asbjørn Slagtern Fjellvåg, UiO, was similar to a classical corrosion mechanism; the grain boundaries serve as a rapid transport path for Pd- and Pt-diffusion, causing the grain boundaries to develop porosity and recrystallize the surface. In short, we can simply describe it as corrosion by platination.
 - ❖ In September, iCSI and NTNU made a contribution to the international catalysis society, by hosting the Webinar for the European Federation of Catalysis Societies (EFCATS) 2021 Catalysis Award event. Eight Award winners were presented, and they all gave lectures showing results from their work. iCSI is proud of our former PhD candidate Dimitrios Pappas, who won the Best PhD Thesis Award.
 - ❖ iCSI is also proud to have dedicated and enthusiastic international scientific advisors. The Annual report introduces the readers to one of the advisors, Professor Regius in Chemistry Graham Hutchings from Cardiff University. Hutchings was the 2021 recipient of the Michel Boudart Award in Fundamental Catalysis from EFCATS and NACS, and iCSI congratulates him on this well-deserved honour!
 - ❖ The representation on the iCSI Board has changed for one of the industry partners in 2021, with Camilla Jordal taking over from Marco Piccinini as Inovyn's board representative in January. We thank everyone on the board as well as all the scientists for their efforts for iCSI throughout the year.

CATHEX lectures

(Advances in heterogeneous CAlysis through integrated THEoretical and EXperimental efforts)

Project organization: Dr. Anne Hoff, Professor Hilde J. Venvik, Associate Professor Jia Yang

The CATHEX project, with support from the INTPART program funded by the Research Council of Norway, is a large network project running from 2020 to 2025. It is linking iCSI with four world-leading catalysis environments: University of Cape Town, South Africa, East China University of Science and Technology, China, University of Toronto, Canada and University of Wisconsin-Madison, USA. The core activity of the network will be to strengthen the integration of theory and experiments in catalysis research and education through personnel exchange and shared workshops. Due to the Pandemic, it was only possible to organize webinars in 2021, but several research exchanges are planned for 2022.



Webinars 2021

Date	Responsible	Title
07.05.2021	Patricia J, Kooyman University Cape Town	Bridging the pressure gap in TEM
21.05.2021	Xingguo Zhou East China University	Regulating the Adsorption Configuration on metal Catalyst for semi-Hydrogenation of Acetylene
04.06.2021	Michael Clays University Cape Town	Catalyst characterization using in situ magnetic measurements
24.09.2021	Hilde J. Venvik NTNU, Trondheim	Methanol partial oxidation to formaldehyde over silver - new kinetic and structural insights
15.09.2021	Magnus Rønning NTNU, Trondheim	Combination of operando characterization techniques for studies of catalyst at industrial working condition
12.11.2021	Anders Holmen, NTNU Jia Yang, NTNU	Studies of the Fischer-Tropsch process Steady-state isotopic transient kinetic analysis on catalysts for Fischer-Tropsch synthesis
10.12.2021	Anja O. Sjøstad University of Oslo	From model to real catalysts operated at relevant process conditions

Ph.D. Candidates and Postdoctoral Projects

Continuous production of liquid jet biofuel from lignocellulose-based feedstocks

Ph.D. Candidate: Albert Miró i Rovira

Supervisor: Prof. De Chen

Co-supervisor: Assoc. Prof. Kumar R. Rout

The transport sector is heavily reliant on fossil-fuels, and it is known that our dependence as society on fossil-based feedstocks is the main source of anthropogenic GHG emissions, that directly contribute to climate change. To help mitigate emissions in the transport sector, alternative fuels and technologies are being developed, e.g., batteries, and fuel cells (powered by H₂). These technologies though, are currently unable to be applied to all fields of transportation, like aviation, where the energy density of these new technologies is far inferior to liquid fuels. Biofuels, in the other hand, is an alternative fuel, that has similar properties to fossil-fuels, and it is already currently blended with traditional fuels, which makes it a convenient replacement to secure the carbon-neutral scenario for this sector.

There are several technologies to produce biofuels from biomass such as gasification, hydrolysis and pyrolysis. Currently, pyrolysis is one of the most promising technologies for liquid fuel production form lignocellulose-biomass. Nevertheless, this process yields a low-quality bio-oil mainly due to a lower energy density, higher corrosiveness and oxygen content compared to traditional fuels. Therefore, to obtain a jet-grade fuel catalytic upgrading of the bio-oil is crucial (Figure 1).

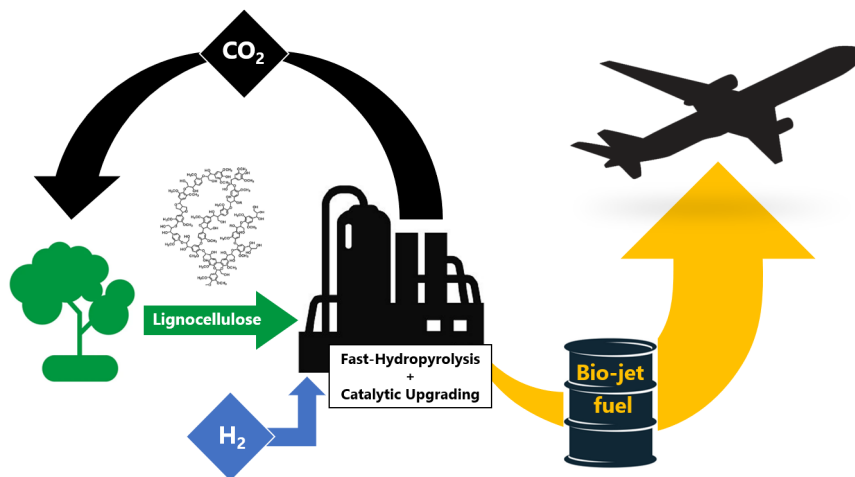


Figure 1. Schematic figure of the chemical upgrading of lignocellulose-biomass to jet-grade fuel

In this project, a mini-pilot plant set-up with both a fast-hydropyrolysis (FHP) reactor and a catalytic upgrading reactor will be used to test several lignocellulose feedstocks for the continuous production of liquid jet biofuel. Several catalysts will be tested for the catalytic upgrading of the pyrolysis-vapors for improving both the energy density and fuel properties of the final product (dual-catalytic carbon coupling and hydrodeoxygenation fixed bed). Furthermore, tuning of operational conditions under a continuous flow high pressure system will be carried out to discern their effects on both FHP and the catalytic upgrading reactions. Additionally, maximization of liquid yield against gas and solid fractions will be evaluated for improving the economic competitiveness of the process.

Financial support:

The project is funded by the Research Council of Norway (NFR) under the Biomass to Aviation Fuel (B2A) project.

Carbon Nanomaterial-Ionic Liquid Hybrid for Ultrahigh Energy Supercapacitor

Ph.D. Candidate: Daniel Skodvin

Supervisor: Prof. De Chen

The desire to use more renewable energy has made energy storage and conversion one of the greatest challenges in today's society. Energy needs to be stored more efficiently, thus improvements in the energy density of supercapacitors (SCs) should be achieved in order to meet today's requirements. The energy density is mainly dependent on the operating voltage window, therefore a lot of time and effort are being used in order to widen the operating voltage window of both SCs using organic electrolyte and SCs using ionic liquid. In this research, mesoporous carbon nanospheres are synthesized and used as electrode material in SCs. This material has a high specific surface area (2000 - 3000 m²/g) and pore volume (1 - 2 cm³/g), which will provide a high ion packing ability and result in a high gravimetric capacitance. In order to increase the operating voltage window (about 2.5 – 3V for organic electrolytes and about 3.5 – 4V for ionic liquid electrolytes), the surface of the carbon material has to be treated. This is because the surface functional groups, mainly oxygen containing groups, can interact with and degrade the electrolyte as the voltage increases. This research is therefore focusing on the correlation between the carbon surface and the performance of the SCs using both organic and ionic liquid electrolytes. The objective is to understand the effect of various functional

groups on the charging and discharging behavior of SCs, which ultimately can result in improvements in the operating voltage window via fine-tuning of the carbon surface. This research has the potential to enable SCs in a wide application range in the energy sector and improve renewable energy storage and conversion. This project could promote the use of renewable energy in the public transportation sector.

Financial Support:

The project is funded by the Research Council of Norway.

Bio-ethanol steam reforming for on board high purity H₂ generation system

PhD. Candidate: Mario Ernesto Casalegno

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 H₂ as an energy carrier can be a sustainable solution that will reduce the impact of human activities on the environment. Provided that H₂ 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 favorable efficiencies to cover energy needs with a significant reduction in greenhouse gas emissions. Steam reforming of hydrocarbons is a mature technology for H₂ production. Bioethanol formed by fermentation processes has significant advantages and appears to be a strong candidate as an energy vector suitable for H₂ production.

Our efforts in this project are focusing on the creation of a prototype that integrates steam reforming of bioethanol for H₂ production with CO₂ separation and H₂ combustion into a compact multichannel reactor that can be used on-board vehicles or marine vessels. 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.

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

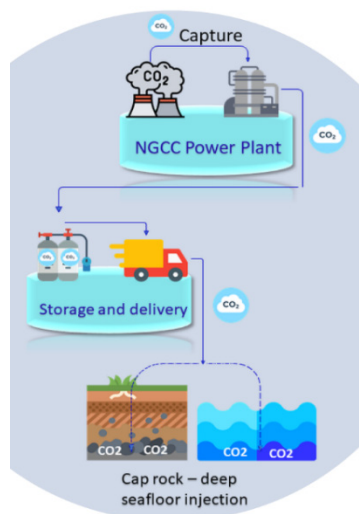
Design of Low-Temperature Carbon Dioxide Adsorbents for Post-Combustion NGCC Power Plant

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 CO₂ 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 CO₂ capture and storage (CCS) (Fig. 1) which is an intensively researched area aimed at mitigating the CO₂ release into the atmosphere. Due to the increase of total natural gas/coal generated electrical power ratio, the project scope is focused on designing CO₂ 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 CO₂. 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 the water is involved only in the chemisorption process and not as a diluent. 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 CO₂ partial pressure and low chemical and thermal stability. Herein, polyethyleneimine (PEI) and pentaethylenehexamine (PEHA) have been used as initial materials for chemisorption. They are described by a very high amine density, which is an important property required to achieve a high CO₂ 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 ($\text{CH}_3 - \text{H}_2\text{N} \cdots \text{H} - \text{NH} - \text{CH}_3$), which minimizes the CO₂

diffusion to the amine sites. The diffusion is also decreased by the high amine loadings. 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 (grafting) concepts are also considered to avoid amine loss.

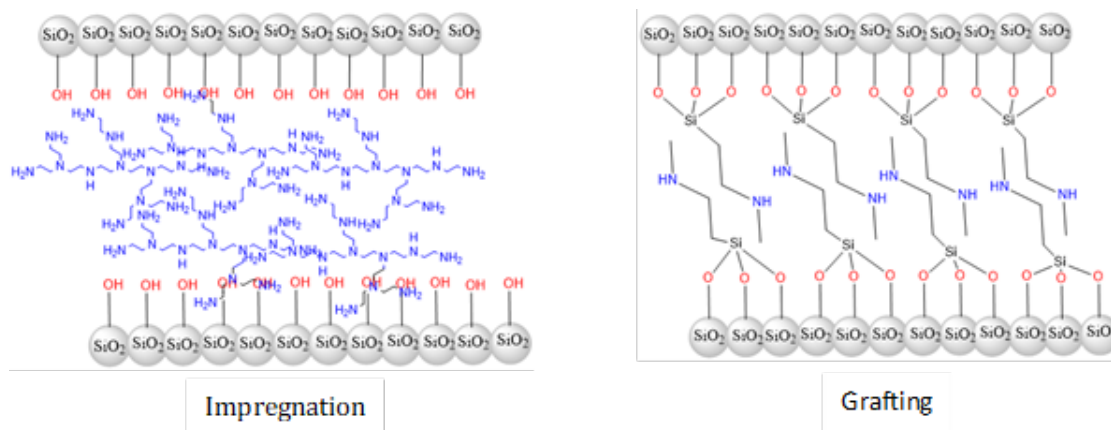


Figure 2. PEI and PEHA impregnation and aminosilane grafting

To store pure CO₂, the adsorption process should be very selective, and the desorption step should be realized in pure CO₂. As the process is designed based on temperature swing adsorption, a desorption step in pure CO₂ and high temperature deactivates immediately the amines, forming ureas compounds. The only type of amine which manifest an extremely good resistance when exposing to these conditions are the one-secondary amine structures. The chemical stability of PEI and PEHA can be also increased by sterically hindering the amines with various bulky structures, however this decreases the capacity, as the bulky structures also inhibit the carbamate formation. Considering this, the project changed the focus to various one-secondary aminoalkoxysilane which can be very easily anchored on the OH-rich silica surface (Fig. 2 -grafting). Besides the impressive chemical stability, the final adsorbent is also thermally stable as the aminoalkoxysilanes are covalently bonded on the support. Since the adsorbent is designed for a post-combustion power plant, it must be resistant to the oxygen present in the flue gas. Long term exposure to oxygen atmospheres at various temperatures is conducted and the deactivation will be investigated through adsorption tests and FT-IR analysis.

Financial Support:

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

Co-pyrolysis of biomass and plastic wastes

Ph.D. candidate: Zhihui Li

Supervisor: Prof. De Chen

Co-supervisor: Assoc. Prof. Kumar Ranjan Rout & Jia Yang

Biofuel which can be produced from biomass is a possible alternative to traditional energy resources. Biomass includes plants, woods, grass, nuts, etc. However, bio-oil directly converted from biomass has a disadvantage of low heating value, corrosion problems, and instability, because of the high oxygen content in the biomass. The oxidation contents can reach 30-60 wt%. These drawbacks of bio-oil can be mitigated by going through the hydrodeoxygenation (HDO) process, however, the HDO method has a high requirement of plants, and the catalysts for HDO are easy to be deactivated due to the coke formation. Thus, it is important to find an easier way to remove oxygen.

Pyrolysis is the main method now to treat biomass, it is thermal cracking under the temperature of 300-600 °C without the presence of oxygen. Pyrolysis can give gas, liquids, and solid main product, coke is the main component of the solid product which is not desired, while the high yield of liquid product that mainly aromatics are expected.

Previous researches found that by mixing hydrogen-rich plastic wastes, for example, polymers from plastic bags, waste tires, etc. with biomass in pyrolysis feedstock, oxygen can be removed by reacting with hydrogen in the form of water (H₂O), which means H rich plastics can play a role as a hydrogen donor, no need for external hydrogen resource to remove oxygen. Compared with HDO method, this way to remove oxygen have fewer requirements on the reactor and catalysts. As previously reported, the heating value of bio-oil can be enhanced from about 14 MJ/kg up to 44 MJ/kg, which is competitive with gasoline (around 45 MJ/kg). Thus, the co-pyrolysis of plastic wastes and biomass have the great meaning of continuing research.

The basic goal of this project is by using co-pyrolysis to convert biomass and plastic wastes into fuels. Different kinds of biomass and plastic wastes will be tested, to find optimal pyrolysis feedstock types and their combination ratios, to produce high quality and quantity liquid bio-oil. Different types of catalysts will be attempted as well, first Y zeolite and ZSM-5 will be attempted as they are the most widely used catalysts for biomass pyrolysis, as well as some other cheap acid catalysts, for example, clay.

Development of stable Cu catalysts for selective hydrogenation of oxygenates

Ph.D. Candidate: Martina Cazzolaro

Supervisor: Prof. De Chen

Co-supervisor: Assoc. Prof. Jia Yang

Catalysts for selective hydrogenation of oxygenates can find application in the upgrading processes of biomass-derived oxygenates streams, i.e. upgrading of bio-oil from biomass pyrolysis, upgrading sugar fractioning products, glycerol conversion. Cu-based catalysts are widely used for selective hydrogenation reactions when C-C cleavage is undesired; although, coking and particles agglomeration and formation of irregularly shaped clusters are common causes of deactivation.

In this project, two sets of catalysts with 5 wt.% Cu loading were prepared: one supported over silica gel; the latter, supported over platelet CNF (PCNF). All catalysts were prepared by incipient wetness impregnation. Silica-supported catalysts were prepared using Cu nitrate, acetate or basic carbonate, dissolved in water, ethanol or isopropanol. Pristine PCNF-supported catalysts were prepared using Cu nitrate or basic carbonate and dissolved in water, ethanol or isopropanol. An additional set of catalysts was prepared with PCNF treated with nitric acid and/or annealing in Ar at 700 or 1000°C, using Cu nitrate and isopropanol for the impregnation. The characterization techniques used were N₂ adsorption, N₂O chemisorption, XRD, TPR, TPD and Raman spectroscopy. Furthermore, the catalysts were tested in the reaction of hydrogenation of hydroxy acetone (HA) to 1,2-propanediol (PD), a model-reaction chosen to define activity, selectivity, and stability. Testing was performed with a fixed-bed lab-scale reactor at 240°C and 6 bar for 48 hours. The catalysts prepared with Cu nitrate were all active and selective to PD, except for the one prepared with PCNF treated at 700°C (without acid treatment). Among these, the most active catalysts were the ones supported over silica and acid and heat-treated PCNF. The catalysts prepared with basic Cu carbonate were all inactive. Lastly, among the ones prepared with Cu acetate, only the one prepared with water showed good activity. Comparing the different sets of catalysts prepared with the same support and precursor, very different trends at varying Cu dispersion were observed. This made us realize the impact that supports, solvents, and precursors have on the activity of the catalysts. Further characterization with XPS and TEM is planned to better understand the nature and contribution of the surface species that could be responsible for the different performances.

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

Ex-situ catalytic upgrading of pyrolysis vapors through supported noble metal catalysts: Process modeling, design and integration.

Ph.D. Candidate: Petter Tingelstad
Supervisor: Prof. De Chen
Co-Supervisor: Dr. Kumar R. Rout

Processes for better upgrading of bio-oils and bio-vapors will be developed through better process design and integration, as well as catalyst development for increased c-c coupling efficiency through Aldon condensation and ketonization reactions, and hydrodeoxygenation efficiency. The main goal will be to reduce the formed non-condensable bio-vapors from 25 % to 10 % thus achieving a higher carbon yield for the product bio-oil as well as enabling a possible source for in-situ hydrogen production. Processes will also be developed to reduce wt% of oxygen in the formed bio-oil, this will be achieved through better catalyst development with focus on increasing the C-O bond stretching of the forming oil, thus facilitating oxygen exit as H₂O, instead of CO₂. The main goal of the project will be to develop processes with higher chemical energy fuel efficiency and yield, as well as reducing the cost of the process while increasing revenues.

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

Multi-Promoter Effect of K, La and Mg in Ethylene Oxychlorination Studied by Operando UV-vis-NIR Spectroscopy

Ph.D. candidate: Wei Zhang
Supervisor: Prof. De Chen
Co-supervisor: Assoc. Prof. Kumar Ranjan Rout

Vinyl chloride monomer (VCM) is a vital chemical as a result of the ever-increasing demand for one of the most commonly used plastic materials, polyvinyl chloride (PVC), through the polymerization reaction.¹ A named as “balanced VCM process” as a highly efficient and environmentally friendly VCM production technology has been widely commercialized around the whole world. Ethylene dichloride (EDC) was firstly formed from ethylene oxychlorination and ethylene direct chlorination,

followed by thermal cracking of EDC to produce VCM, accompanied by consuming HCl recycle to participate in ethylene chlorination and close the chlorine loop.²

CuCl₂/γ-Al₂O₃ -based catalyst is the most used in industrial process due to the outstanding EDC yield. It is widely accepted that CuCl₂ catalysts based on a Mars-van Krevelen (MvK) mechanism is a three-step redox cycle, including the reduction, oxidation, and hydrochlorination steps.¹ However, a fast deactivation due to particle agglomeration and vaporization of CuCl is still the main challenge for the commercial catalyst, which is related to the Cu⁺ concentration of the catalyst. Therefore, promoters such as alkali, alkali earth, and rare-earth metals (like K, Na, La, Mg, etc.) are used as the promoters to accelerate the oxidation of CuCl to form more CuCl₂ and inhibit the copper loss. The higher CuCl₂ concentration is the key factor for high activity, selectivity, and stability in ethylene oxychlorination.³

UV-vis-NIR spectroscopy is widely used in the research on transition metal ions. In our previous report, a linear relationship between the total CuCl₂ concentration of catalyst and the normalized KMF (NKMF) units for the reduction and oxidation steps was obtained. The value of KMF at 793 nm is sensitive to the d-d transition band, while CuCl with the electronic configuration of 3d¹⁰, does not exhibit a d-d band transition.¹ Therefore, a decrease of CuCl₂ on the catalyst, accompanied by an increase of CuCl, results in a decreasing KMF as the reduction proceeds.

In this work, γ-Al₂O₃ supported different metals K-, La- and Mg-doped CuCl₂ catalysts were prepared by the incipient-wetness impregnation method. A relatively simple operando, namely combined GC and UV-vis-NIR was utilized to study the multi-promoter effect and elucidate the timely and spatial distribution of the Cu species with the catalytic performance. The steady-state performance of the catalyst in the relatively low and high conversion regions were studied due to the very high conversion in industry and the performance of catalysts may be linked to the conversion level.

The results indicated that three metals doped KLaMgCu/γ-Al₂O₃ catalyst has the highest activity and selectivity over both low and high conversion ranges. At steady state, the CuCl₂ concentration distribution along the catalyst bed of KLaMgCu/γ-Al₂O₃ catalyst was much higher than the other three CuCl₂ based-catalyst, indicating this catalyst had a great effect on improving the CuCl₂ concentration and enhancing the activity, selectivity, and stability. XPS of the four different metal-doped catalysts was also carried out to illustrate the electronic property of Cu species modified by multi-promoter doping. Clearly, as the promoter doped, the proportion of Cu²⁺ on the catalyst gradually increased, implying that KLaMgCu/γ-Al₂O₃ has the ability to maintain a higher oxidation state. This study is expected to provide one way for exploring the potential benefits of multi-promotion on CuCl₂/γ-Al₂O₃-based industrial oxychlorination catalysts to improve the catalytic performance and understand the reaction further.

Financial support: This work was supported by the industrial of Catalysis Science and Innovation (iCSI), a center for Research-based Innovation funded by the Research Council of Norway under the grant No. of 237922.

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Moving Bed Carbonate Looping (MBCL), Phase III

Participants: Prof De Chen (NTNU), As. Prof. II Kumar R. Rout (NTNU-SINTEF), Torleif Madsen (FTG), Asbjørn Strand (FTG), Ainara Moral Larrasoana (NTNU), Anne Charlotte Wold (NTNU), Eirik Giil Woxholt (NTNU)

The moving bed carbonate looping concept (MBCL) was developed by NTNU/SINTEF/FTG since 2017. In the project MBCL phase I and II, a conceptual design of a MBCL plant was proposed, with special design of carbonator moving bed reactor to handle large flue gas from the NGCC power plant (Fig 1). The philosophy has been to reduce the reactor size, cost and energy consumption for post-combustion CO₂ capture by the combined use of process intensification, i.e., by developing optimized process design, cheaper solid sorbents, the compact reactor and easy operation.

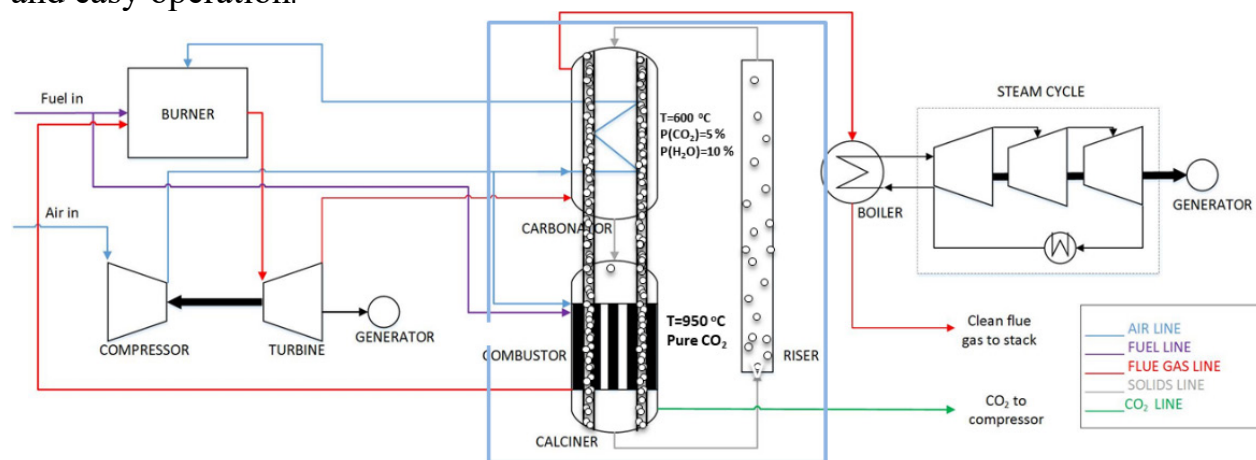


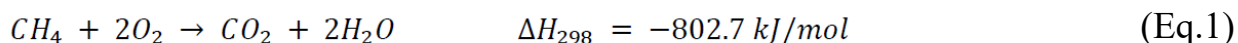
Fig. 1. Process flow diagram for the Hybrid NGCC with PCCC through CaL in MBCL

In CLIMIT project MBCL phase I and II, the concept of heat integration to calciner was carried out by the catalytic combustion, where doped dolomite pellets (DDP) were considered, and process efficiency were calculated using ASPEN. It was found that the energy efficiency of NGCC power plant with PCCC by MBCL is 55.8% points, whereas the NGCC plant without CO₂ capture is 57.6% point, as reported by MBCL phase I. The energy penalty of CO₂ capture by MBCL is about 1.8% excluding CO₂ compression, which correspond to the best efficiency and lowest of energy penalty that is ever published for NGCC power plant integrated with PCCC. It is noted that proper heat integration is essential to increase the energy efficiency of the power plant.

The Cost evaluation of MBCL plant, i.e., CAPEX and OPEX was done and compared with conventional MEA plant. The MBCL system can decrease annual cost by 32.2% and the net cost of CO₂ avoided is reduced by 42.4% in comparison to MEA system. A sensitivity analysis was done by varying the important cost parameters, i.e., increasing contingency, sorbent make-up, operational cost by 100% and increasing the MBCL plant energy penalty two-fold, it is found that the MBCL still would be a preferred technology in comparison to MEA technology.

Extensive research has been done before in order to produce a cost-efficient chemically stable solid sorbent including our effort to our previous patent (NTNU). However, additionally to the challenging chemical degradation of the natural calcium oxide-based sorbents, that has been mainly discussed of the Phase I and II in the MBCL project, the mechanical degradation due to mainly attrition and abrasion, caused by the motion of the solid provoking the collision of the particles between them, as well as with the walls of the reactors and the riser, must be analysed. In the phase III of the project the examination of the attrition behaviour of the pellets has been studied by means of and standardized measurements (ASTM-D5757-00), as well as the compressive strength of the individual pellets, along with an attempt of improving the mechanical strength by a 2nd generation sorbent in order to improve the mechanical properties of the pellets.

Furthermore, in Phase I and II, in the MBCL technology, the heat required in the calciner is proposed to be provided by the burning of Natural Gas (Eq.1) in a fixed bed catalytic combustor placed outside of the moving bed calciner and therefore, avoiding the direct gas/solid contact.



In the Phase III of the MBCL project hard efforts has been made in order to validate the used of the catalytic methane combustion for the heat supply in the calciner. Fig

2 shows the installation designed to validate the heat exchanger proposed in the project.

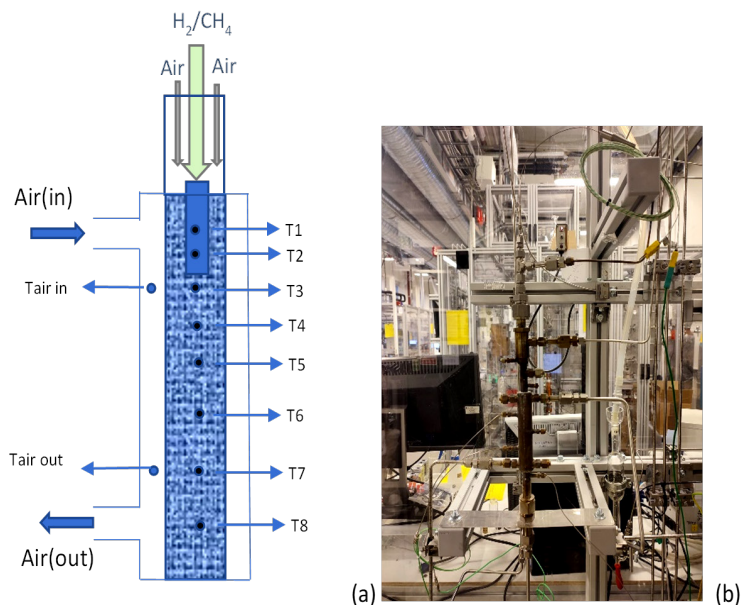


Fig. 2. Methane combustion reactor and heat exchanger

Financial support: GASSNOVA

Kinetic Studies of Ethylene Oxychlorination to Ethylene Dichloride and Vinyl Chloride

PostDoc: Hongfei Ma
Supervisor Prof. De Chen

Polyvinyl chloride (PVC) is the most versatile of all thermoplastics that can be used in a wide range of applications. It is the third-highest volume polymer, slightly behind polyethylene and polypropylene. Vinyl chloride (VCM), the monomer of PVC is the key building block for PVC production, which is mainly produced from ethylene dichloride (EDC) through thermal cracking. Currently, approximately 90% of VCM production plants worldwide are using a balanced VCM process where Cl₂ by first chlorinating ethylene to produce EDC, the EDC is then thermally converted to VCM. The HCl produced in the dehydrochlorination reactor is typically captured and recycled to an oxychlorination reactor to convert C₂H₄, O₂, and HCl to EDC, which is again converted to VCM. EDC dehydrochlorination also called EDC cracking, is an energy-intensive process, which is carried out at high temperatures (500–550 °C), high pressures (15–20 bar), at a conversion of approximately 50–60%

leading to an overall VCM yield about 50% in a single pass. The complexity of the process drives a search for simplifying the process to produce VCM directly from C₂H₄, O₂, and HCl in a single pass reactor.

An easy operando method combining UV–vis-NIR and mass spectroscopy was developed to elucidate the active sites, rate-determining step, and predict the reaction rate and Cu oxidation state at the steady-state by the rate diagram. The influence of the promoters can be reflected by the reduction and oxidation rates, and the intersection point can be used to evaluate the catalysts behavior.

Process optimization needs a reliable model since catalysis is a kinetic phenomenon. Especially, ethylene oxychlorination is following the Mars–van Krevelen mechanism, and the catalyst partakes the reaction. The chemical state and the concentration on the catalyst surface are dynamic changes during the reaction process. Therefore, a kinetic model with an accurate description of the active component changes is highly desired. We reported two kinetic models on this Mars–van Krevelen mechanism considering the dynamic changes of the active sites utilizing combined transient and steady-state kinetic study. The proposed kinetic model can accurately describe the catalytic behaviors of the half-reactions of reduction and oxidation steps.

We have demonstrated an efficient method for produce VCM in one single-step at relatively low temperature and pressure on a metal-free carbon catalyst. A reaction mechanism of Cl-loop between ethylene oxychlorination and EDC dehydrochlorination was proposed and to rationalize the observed synergy effect of the two reactions. We also utilized the dual-bed configuration method to produce VCM with a much higher yield than the current two-step industrial process in a single-pass.

These findings are supposed to provide not only the fundamental understanding of the nature of ethylene oxychlorination from both experimental and DFT studies but also the way for rational catalyst design for the future. A metal-free carbon-based catalyst was proposed to have a significant impact on the VCM-related studies toward a more cost- and energy-effective process.

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

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Fundamental understanding of ethylene oxychlorination catalysts by DFT — Effects of different promoters

Postdoctoral fellow: Yalan Wang
Supervisor: Prof. De Chen

Ethylene oxychlorination is an important process to produce ethylene dichloride (EDC), vinyl chloride monomer (VCM) and polyvinyl chloride (PVC). $\text{CuCl}_2/\gamma\text{-Al}_2\text{O}_3$ is identified as a superior catalyst for ethylene oxychlorination. However, the $\text{CuCl}_2/\gamma\text{-Al}_2\text{O}_3$ 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 catalyst to maintain and enhance the catalyst stability and activity. Although the addition of promoters exhibits better performance, the exact mechanism of the promoter effect remains unclear. In this work, DFT calculations are used to gain insight into the promoter effect, with LiCl , NaCl , KCl , RbCl , CsCl , BeCl_2 , MgCl_2 , CaCl_2 , SrCl_2 , BaCl_2 , and LaCl_3 as promoters on $3\text{CuCl}_2/\gamma\text{-Al}_2\text{O}_3(110)$. The catalyst surface with 1 Cl vacancy is selected as starting surface due to the existence of Cl vacancies on the catalyst surface under realistic reaction conditions.

The three-step redox mechanism of ethylene oxychlorination, which includes reduction, oxidation, and hydrochlorination, has been calculated on above catalyst surfaces. The three-step redox mechanism on the group IA elements, namely Li-, Na-, K-, Rb-, and Cs-doped catalysts was calculated firstly. It is found that addition of Na, K, Rb, and Cs reduces the O_2 dissociation barrier, but increases reduction barrier. Addition of Li reduces both reduction and oxidation barriers. The RDS is changed from O_2 dissociation to EDC desorption for Li-, Na-, K-, Rb-, and Cs-doped catalysts. Both reduction and oxidation barriers are found to be correlated with formation energy of Cl vacancy, further related to charge of Cl and promoter ionization energy. Subsequently, the kinetic equation is obtained from kinetic analysis, based on that the catalyst activity is calculated as turnover frequency (TOF). Meanwhile, the catalyst stability is calculated as removable CuCl_2 concentration. Both charge of Cl and promoter ionization energy can be used as descriptors to probe catalyst activity and stability. Li-doped catalyst exhibits higher activity and stability than undoped catalyst among group IA elements.

The three-step redox mechanism was then calculated on Be-, Mg-, Ca-, Sr-, Ba-, and La-doped catalysts. Addition of Be, Mg, Ca, Ba, and La reduces the O_2 dissociation barrier, but increases reduction barrier. Addition of Sr increases both reduction and oxidation barriers. The RDS is changed from O_2 dissociation to EDC desorption for all doped catalysts. Promoter ionization energy can be used as descriptors to probe catalyst activity and stability. CuCl_2 stability is increased by

doping all investigated promoters. Mg- and Be-doped catalysts display higher activity and stability than undoped catalysts. The calculation gives the insight of promoter effect on $\text{CuCl}_2/\gamma\text{-Al}_2\text{O}_3$ catalyzed ethylene oxychlorination.

Financial support: The project is funded by Center for industrial Catalysis Science and Innovation (iCSI), which receives financial support from the Norwegian research council.

Catalytic Steam Reforming of Hydrocarbon Impurities from Biomass Gasification

Ph.D. candidate: Ask Lysne

Supervisor: Prof. Edd A. Blekkan

Co-supervisor: Kumar R. Rout

Renewable energy sources like hydroelectric, wind and solar power can provide vital low-emission electricity. The electrification of some industrial and transportation niches is however limited by the considerably lower energy density and recharging efficiency compared to liquid fuels. Integration of biomass gasification and Fischer-Tropsch (FT) synthesis in biomass-to-liquid (BTL) technology is an attractive option for production of high-quality renewable liquid fuels. Successful integration of these technologies 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 as well as the adjustment of $\text{H}_2/\text{CO}/\text{CO}_2$ ratio. The elimination of condensable hydrocarbons (tars) is considered to be the most cumbersome challenge of the commercialization of such processes.

The PhD project is addressing catalytic steam reforming, converting hydrocarbon impurities from biomass gasification to useful gas products as part of this key syngas cleaning step. Simultaneous $\text{H}_2/\text{CO}/\text{CO}_2$ ratio adjustment by the WGS reaction, preparing the syngas for downstream FT synthesis, is also demonstrated. Bi-metallic Ni-Co/Mg(Al)O catalysts have been prepared by calcination of hydrotalcite precursors and tested for tar model (toluene) removal at relevant operating conditions. The fresh catalysts are characterized by ICP-MS, XRF, powder XRD, TPR, N_2 -chemisorption and H_2 -physisorption. The effects of key parameters like Ni-Co ratio on coke morphology and location is studied by TGA-TPO, Raman spectroscopy and SEM/EDS after steam reforming operation.

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

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 of the oxidation of NO to NO₂ over different catalysts (based on noble metals or base metal oxides). The conditions are chosen to emulate typical industrial conditions, moderate pressures and T in the range 150–450 °C. The experiments involve switching from ¹⁴NO + O₂ to ¹⁵NO + O₂ to study the N-containing pathway as well as from NO + ¹⁶O₂ to NO + ¹⁸O₂ to study the O-containing pathway in the formation of ¹⁴N¹⁶O₂, ¹⁵N¹⁶O₂ as well as N¹⁶O¹⁸O and N¹⁸O₂ products respectively. These results give insight into the mechanism and properties of the catalysts. One approach is to use the single-pool model [2] to analyze the data from the experiments and use this to estimate the abundance, surface coverage and the mean residence time (surface lifetime) of reaction intermediates. The idea is to use this information to discriminate between the dominant mechanism of reaction; either a Langmuir-Hinshelwood type or an Eley-Rideal type, 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, and this information is used to probe the nature of active sites of the catalyst. With these fundamental experimental data, it will be possible to have a better understanding of the catalytic reactions and thereby use the data for better catalyst design

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

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Conversion of synthesis gas from biomass gasification over cobalt catalysts

Ph.D. Candidate: Oscar Ivanez

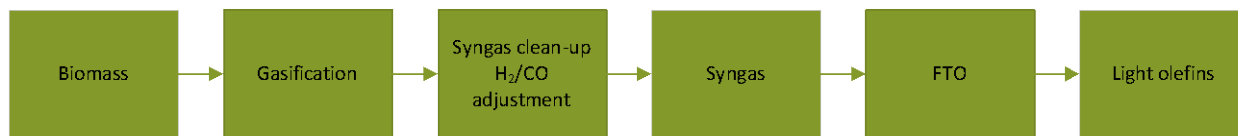
Supervisor: Prof. Edd A. Blekkan

Co-supervisor: Kumar R. Rout

The increasing development of the global industry demands further energy production. The main source of energy are the fossil fuels, and their use has been increasing every year. In 2016, more than 80% of primary energy in the world was provided by fossil fuels. The new policies and future scenarios, where the increased prices of the fossil fuels and the demand of cleaner fuels, make necessary alternatives of fuel production.

Biomass to liquids via gasification and Fischer-Tropsch synthesis (FTS) is an interesting alternative for fuels and chemicals production. Among the FT products, light olefins represent added value compared to fuels, which always will be the main product. Ethylene, propylene and C₄ fractions, mostly produced by cracking in the refineries, are key building blocks in the petrochemical industry. There are however alternatives based on the conversion of syngas into olefins. FTS to olefins has the potential of reducing the overall cost by the direct production of light olefins without intermediate steps.

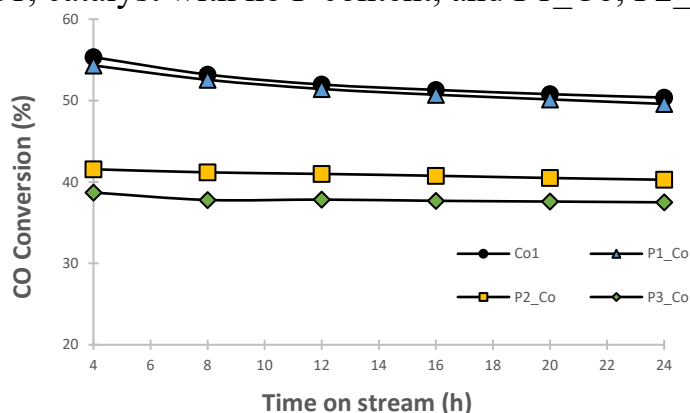
Via gasification, biomass has the potential to be a source for hydrocarbon products, due to feedstock flexibility and the possibility to reduce net CO₂ emissions. The syngas can be produced from different sources such as natural gas, coal or biomass. Biomass is an abundant and renewable energy source and source of carbon. The process also opens the possibility to improve the total yield of different



industries by using waste as a feedstock for the FTS. Examples of such industries are forestry, agriculture and aquaculture. The total aquaculture production in Norway in 2018 was 1.354.941 tons, with 68% of the amount being edible. This represents an opportunity to valorize the fish waste in order to reduce the economic losses and improve the efficiency of the industry.

Furthermore, biomass conversion via gasification opens the possibility of using waste as a feedstock for the chemicals and fuels. However, to produce light olefins via FTS from biomass, it is necessary to clean-up and adjust the composition of the syngas. Several inorganic species such as alkali and alkaline earths metals, P, Cl, nitrogen compounds etc. can be present in the syngas.

In this context, the objective of this work has been the investigation of the effect of the deposition of different contaminants in cobalt-based catalysts in the FTS in conditions favoring light olefin production. Four different cobalt-manganese-based supported on alumina catalysts were prepared with increased phosphorus content, named Co1, catalyst with no P content, and P1_Co, P2_Co and P3_Co.



The addition of phosphorus leads to a high degree of deactivation, decreasing the intrinsic activity, the C₂₋₄ olefins and C₅₊ content and increase the methane and linear hydrocarbons selectivity, implying a higher degree of hydrogenation.

Financial support: The project is funded by the Center for Environment-friendly Energy Research (FME) Bio4Fuels

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

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 H₂, CO, CO₂, H₂O, CH₄, H₂S 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 in thermochemical conversion processes.

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.

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Surface chemistry of sputtered Pd alloy membranes 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 and uses, hydrogen purification is a crucial step to the successful implementation of hydrogen energy systems. Pd-based membranes 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 H₂ separation on a side stream of the Equinor Methanol plant at Tjeldbergodden, Norway. Ultra-pure H₂ is produced, while at the same time, CO₂ can be captured and stored.

Typical mixture gases 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. CO₂ has little impact by competitive adsorption, but its total effects on the surface reaction chemistry remain to be understood. NH₃, as a potential C-free energy storage and carrier, should also be taken into consideration. Its 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 needs to be studied.

This PhD project mainly focusses on the thermochemical factors critical to separation performance and long-term stability. The membrane performance test-rig has been renovated and mixture experiments are ongoing. The effect on 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 H₂MemX (Enabling ultrathin Pd based membranes through surface chemistry diagnostics and control) project is funded by the Research council of Norway ENERGIX program (grant 280903).

Partial oxidation of methanol to formaldehyde over silver

PhD Candidates: Youri van Valen

Supervisor: Prof. Hilde J. Venvik

Co-supervisors: Senior Researcher Dr.ing Rune Lødeng (SINTEF), Associate Professor Jia Yang.

As part of iCSI we are looking into the partial oxidation of methanol to formaldehyde over a silver catalyst. Formaldehyde is a base chemical that has a variety of applications, notably in the production of wood adhesives and fine chemicals. Together with partners Dynea AS, K:A: Rasmussen, and SINTEF we aim to gain fundamental knowledge on the MTF process and the silver catalyst. The main objective is to use this knowledge to increase the overall yield of the process and increase the catalyst lifetime.

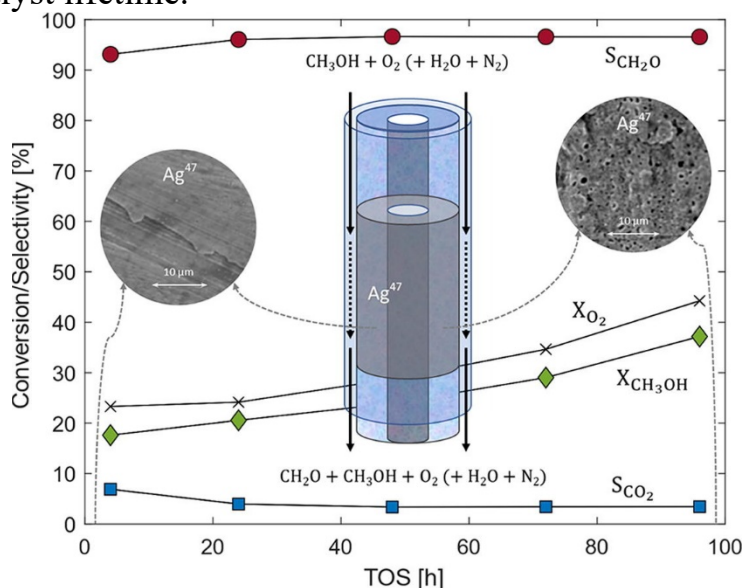


Figure: Graphical abstract of Lervold et al. (2021) showing the conversion plots (marked X) and selectivity plots (marked S), a schematic representation of the annular catalyst fitted in the reactor, and the development of the silver surface over the course of the MTF reaction.

In 2021 Stine Lervold concluded her PhD on this project. During her project an annular reactor design was developed and implemented. This reactor design has

enabled running the MTF reaction at partial oxygen conversion at industrially relevant temperatures by solving challenges such as gas phase reactions and mass transfer limitations. This allowed for the extraction of kinetic data. The graphical abstract of the final publication of her PhD is shown in figure 1. Formaldehyde selectivity up to 97% was obtained.

For the continuation of the project, we have been looking at the interaction between the silver catalyst, oxygen, and some of the sub-reactions of the MTF reaction. By looking at CO and H₂ oxidation we have observed that the reaction atmosphere the silver catalyst has been exposed to can have a significant effect on the catalytic properties of the metal. This ‘catalyst history’ has provided an interesting avenue to explore for further research, and coupling to relevant characterisation data is the next challenge to tackle. To this end we have been and will continue to utilize advanced characterisation techniques within iCSI, such as TEM, and have had an excursion to MAXIV for *in situ* X-ray ptychography. The results from these and coming experiments will be shared within iCSI to aid R&D activities into this process, and eventually published.

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).

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

Researchers: Dr. Mehdi Mahmoodinia, Dr. Marie Døvre Strømsheim.

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

Understanding the dynamic surface of a cobalt (Co)-based Fischer Tropsch (FT) catalyst motivated this work with Co single crystals. The active phase of industrially applied catalysts consists of metallic Co nanoparticles that expose a heterogeneous surface with a large variety of active sites (corners, edges, steps, kinks, reconstruction), and a fundamental understanding of adsorbates on different Co sites was therefore targeted by the investigation of three different single crystal surfaces: Co(0001), Co(10-12) and Co(11-20). A combination of density functional theory (DFT) study, temperature programmed desorption (TPD) and low electron energy diffraction experiments have been used in collaboration with Dr. Kees-Jan (C.J.) Weststrate at the SynCat@DIFFER research lab in Eindhoven, the Netherlands.

An important elementary step in FT synthesis is the dissociative adsorption of H₂ on the Co surface to enable further hydrogenation. Our results demonstrate that the influence of surface structure on the adsorption and dissociation of hydrogen is surprisingly large. The TPD data show lower hydrogen desorption temperatures on the more open surfaces. This is in agreement with the results from the DFT calculations, finding that hydrogen adsorbs weaker on the corrugated (11-20) and (10-12) surfaces compared with the flat (0001) surface. The lateral interactions between adsorbed hydrogen atoms were also obtained from calculations with sequentially increased hydrogen coverage, and the results were qualitatively in line with the trend in TPD desorption temperatures for the three surfaces. In the context of hydrogenation of CO over supported Co particles, our study agrees with previous work suggesting that undercoordinated Co sites are important for efficient H₂ dissociation. After dissociation, diffusion of hydrogen atoms to sites with higher adsorption strength on the flat terrace is facile, making it available for hydrogenation reactions.

The combined DFT and TPD investigation of the CO-induced (3×1) reconstruction of the surface of Co(11-20), previously studied by Venvik et al. with scanning tunneling microscopy (STM), sought to elucidate the species migrating during the reconstruction as well as the structure of and adsorption site of CO on the reconstructed surface. The CO TPD results showed only a minor difference in the desorption peak temperature, with the reconstructed surface having the highest desorption temperature. Two theoretical model surfaces with (3×1) periodicity were compared to the unreconstructed surface, one with a missing and one with an added, [0001]-directed, zigzag row of Co atoms. The DFT results inferred that the added row structure is energetically preferred under CO exposure, with CO adsorbed on the rows in the top layer of the reconstructed surface. The assumption from the previous work that the migrating species is a cobalt carbonyl was also supported.

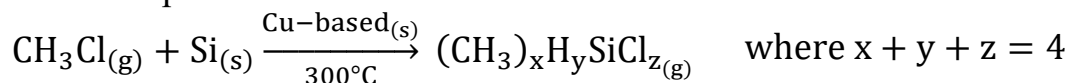
Financial support: The research has been performed with support from the Department of Chemical Engineering, NTNU, and the Research Council of Norway under the contracts 280903, 237922 and 174893/O30, and Equinor ASA through the Gas Technology Centre (NTNU-SINTEF) and NTNU. The computations were performed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

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:



The dominant and main product of interest in this process is dimethyldichlorosilane, $(\text{CH}_3)_2\text{SiCl}_2$. 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.

Transmission electron microscopy (TEM) characterisation of catalyst materials

Postdoc: Tina Bergh

Advisor: Prof. Hilde J. Venvik

The postdoctoral work concerns electron microscopy characterisation of various materials, by using (scanning) transmission electron microscopy ((S)TEM) in particular. (S)TEM enables atomic resolution imaging of materials, and offers the possibility of studying the morphology, chemical composition, and crystal structure in the same sample volume using only one instrument. The postdoctoral position has received funding from several sources, including the SFI iCSI, IKP and the project AluBridge, which facilitates collaboration on a broad range of materials characterisation projects. The focus is placed on developing new or improved methodologies for (S)TEM characterisation, including topics such as sample preparation, in-situ heating and gas reactions, data collection and data analysis. When it comes to the data collection and analysis, there is a special interest towards scanning electron diffraction data.

Within iCSI, the work was mainly devoted to characterisation of silver catalysts used in the methanol to formaldehyde reaction, in collaboration with PhD candidate Youri van Valen and others. The silver catalyst undergoes massive restructuring as it interacts with oxygen at high temperature, and ongoing research concentrates on further understanding these structural changes. TEM lamellae were fabricated by focused ion beam (FIB) lift-out. Figures 1(a)-(d) and 2(a) show secondary electron (SE) scanning electron microscopy (SEM) images acquired during FIB lamella preparation, while Figures 2(b)-(e) show various TEM images of a finished lamella.

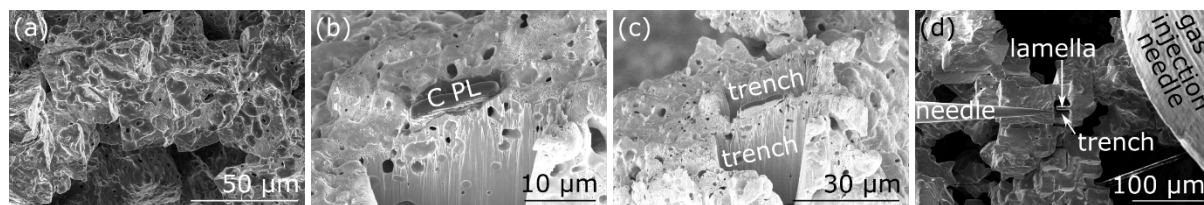


Figure 1: SE SEM images acquired during FIB preparation of a TEM lamella from a silver particle. The silver particles were produced by K.A. Rasmussen and had been exposed to lab scale methanol to formaldehyde synthesis conditions. (a) shows the typical morphology of used silver particles. (b) shows a carbon (C) protection layer (PL) deposited on the surface of a silver particle, while (c) shows the same particle after milling of trenches using the FIB. (d) overview image where a needle that was used to transfer a lamella to a TEM grid can be seen, together with the gas injection needle that was used for C deposition.

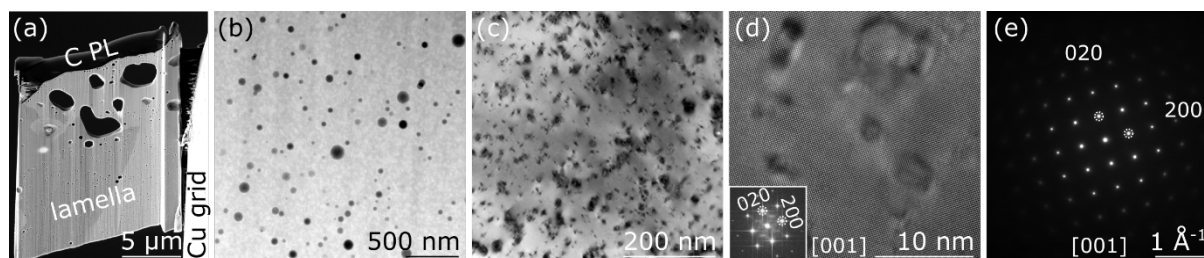


Figure 2: Characterisation of silver particles that had been exposed to lab scale methanol to formaldehyde synthesis conditions. The particles were produced by K.A. Rasmussen. (a) SE SEM image of a lamella attached to a Cu TEM grid. (b) High angle annular dark field-(HAADF-)STEM image showing pores found within the silver. (c) Bright field-(BF) TEM image where the strain fields from crystal defects can be seen. (d) High resolution-(HR-)TEM image acquired from silver oriented to zone axis [001], where the bottom left inset shows the central part of the fast Fourier transform of the image. (e) Selected area electron diffraction (SAED) pattern from a single crystalline silver region oriented to zone axis [001].

Further, TEM characterisation was performed of copper (Cu)-based lignin catalyst materials, in collaboration with Postdoc Hongfei Ma and Prof. De Chen. The focus was placed on studying the presence of Cu or Cu-containing particles within the samples. PhD candidate Joakim Tafjord and Assoc. Prof. Jia Yang work on the development of novel iron (Fe)-based catalysts for the Fischer-Tropsch synthesis. TEM characterisation of these catalysts was initiated, and proof-of-concept trials were done with the aim of developing an inert sample transfer routine by conducting sample preparation within a glove box. Collaboration was also started with Postdoc Katarzyna Swirk, advised by Prof. Magnus Rønning, who works on Ni-based mesoporous silicas from rice husk ash for tri-reforming of methane. The material was characterised by TEM with the main focus placed on studying the distribution of the various elements contained within the samples.

Financial support: The postdoctoral position is supported 50% by the National Centre for Research-based Innovation (SFI) Industrial Catalysis Science and Innovation (iCSI) (RCN 237922) IIA6, 25% by the Department of Chemical Engineering (IKP), and 25% by the BIA project AluBridge (RCN 314063).

***In-situ* analysis of industrial catalytic reactions using a novel In-situ Mass Analyzer (ISMA)**

Ph.D. Candidate: Björn Frederik Baumgarten

Supervisor: Associate Professor Jia Yang

Co-Supervisors: Prof. Edd A. Blekkan, Prof. De Chen, Senior Researcher Rune Lødeng

For many industrial reactions, the formation of coke (or other deposits) is a relevant side reaction which leads to deactivation of the catalyst. With the ISMA, deposition kinetics and deactivation kinetics can be investigated simultaneously. In addition, sorption processes can be investigated.

The ISMA is an ideal plug flow fixed-bed reactor with the added ability to simultaneously measure the weight changes of the catalyst bed during reaction. The reactor tube is oscillating, and the frequency is correlated to the mass via a spring constant. Thus, the mass of the catalyst can be recorded in real time during the reaction.

The time resolution of the mass signal is about 0.1 s, with a sensitivity of about 1 µg. The reactor has a volume of 200 to 900 µl, and the feed section is equipped with a liquid flow controller and 8 mass flow controllers for different gases. The reactor can be pressurized up to 62 bar at temperatures of up to 700 °C, covering a wide selection of industrial reaction.

Interesting areas for the ISMA are CO₂ sorption processes, Methanol to Olefins, Fischer-Tropsch synthesis, and many more. After installation of the ISMA, first, it will be used to investigate CO₂ sorption, before it will be used for more challenging processes involving chemical reactions like Fischer-Tropsch synthesis and coupled CO₂ hydrogenation and MTO. Additionally, depending on the predictability of the influence of changing temperature on the weight signal, thermogravimetric analysis might be an interesting application due to the defined flow through the sample.

The ISMA was developed and will be provided by SINTEF. It is an improved version of the earlier TEOM (Tapered Element Oscillating Mass balance). This project is pioneering and the first to demonstrate the instruments capabilities at relevant conditions.

Financial support: The project is a research activity (IIA6 WP6.6) 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)

Utilization of alginate for the synthesis of carbon-supported catalysts

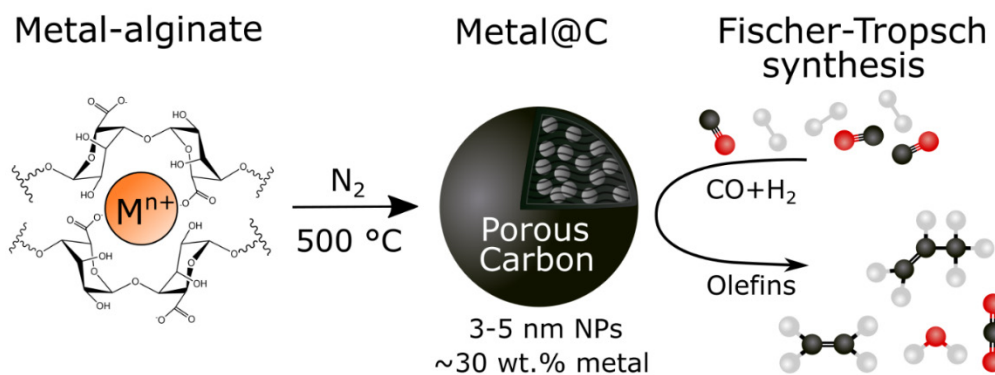
Ph.D. Candidate: Joakim Tafford

Supervisor: Assoc. Prof. Jia Yang

Co-supervisors: Prof. Em. Anders Holmen, Prof. Em. Erling Rytter and Research Scientist Rune Myrstad

Lower olefins (C_2 - C_4) and their derivatives are important building blocks in the chemical industry but are mainly produced from petroleum-based feedstocks. An alternative production route is through the Fischer-Tropsch synthesis (FTS). In this reaction, syngas ($CO+H_2$) react to form valuable chemicals and fuels. Iron catalysts have low hydrogenation activity and are operated at high temperatures (300 – 350 °C), which makes it the catalyst of choice for C_2 - C_4 olefins. Having high water-gas shift activity is also desirable when the syngas is produced from hydrogen lean feedstocks such as coal or biomass, removing the need for upstream hydrogen adjustment.

This project aims to employ alginate, an abundant biopolymer found in brown algae, as a carbon precursor for the synthesis of novel catalysts. Metal-containing alginates are subjected to pyrolysis to produce well-dispersed metal nanoparticles supported on porous carbon. The investigated metals are Fe, Co, Ni, and Cu, but the main focus is on Fe-catalysts. The synthesis and pyrolysis conditions are investigated and tuned to achieve material characteristics that are suitable for highly active catalysts. The properties are optimized to attain high catalyst stability, activity, and selectivity towards lower olefins in the Fischer-Tropsch synthesis. These investigations require a wide array of characterization techniques, many of which are *ex situ* measurements (XRD, BET, TGA, TEM, FTIR, Raman spectroscopy). They also encompass *in situ* investigation (FTIR, XAS, XRD), and *operando* measurements (XAS, XRD, Mössbauer) to study the pyrolysis process, the effect of different catalyst activation procedures, and how the addition of promoters affect the catalyst characteristics and performance.



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

Bismutite-based Hybrid Nanoparticles for Enhanced Visible Light Photocatalytic Degradation of Organic Pollutants

PhD candidate: Jibin Antony

Supervisor: Magnus Rønning

Co-supervisors: Jia Yang, Sulalit Bandyopadhyay

Semiconductors which can be activated under sunlight have attracted intense research interest due to their applications in heterogeneous photocatalysis, especially in the degradation of organic pollutants. Bismutite ($\text{Bi}_2\text{O}_2\text{CO}_3$, BSC) nano discs (NDs) have recently emerged as an important candidate in photocatalysis due to its alternate $(\text{Bi}_2\text{O}_2)^{2+}$ and CO_3^{2-} layered anisotropic crystal structure and internal static electric field, which facilitates photoinduced charge transfer and separation. Previous works have reported BSC as an efficient photocatalyst in the degradation of organic dyes such as methylene blue, methyl orange and rhodamine B. However, its use has primarily been limited to the UV spectrum due to the relatively wide bandgap of 3.12 eV. Hence specific tailoring of properties of a photocatalyst is important for improved light harvesting and faster mineralization of organic contaminants leading to better solar energy conversion efficiency.

Due to its porous structure and high surface-to-volume ratio, silica has attracted attention as a good adsorbent. Improved adsorption of cationic dyes has been reported in presence of silica due to electrostatic and hydrogen bond interactions with the large amount of silanol groups present on surface. In addition, silica has also been reported to introduce defect states associated with oxygen vacancies in semiconductors. On the other hand, gold nanoparticles (Au NPs) owing to their excellent optical properties and localized surface plasmon resonance (LSPR) effect, have emerged as attractive candidates for catalysis. As a result of the LSPR effect, enhanced field strength of the electromagnetic fields near the surface of Au NPs can be much larger than the applied field for structures with sharp edges. Since different shapes of Au NPs would absorb light at different regions of the electromagnetic spectrum, depositing these NPs on semiconductor substrates would enhance the light harvesting properties of the hybrid.

In this project, different approaches to improve the photocatalytic activity of BSC under sunlight/visible light such as modification with a good adsorbent with simultaneous incorporation of defect states, deposition of anisotropic gold

nanoparticles etc. would be carried out. Furthermore, to be able to quickly retrieve the catalyst after the reaction, strategies to introduce a magnetic core into these hybrid photocatalysts will also be investigated.

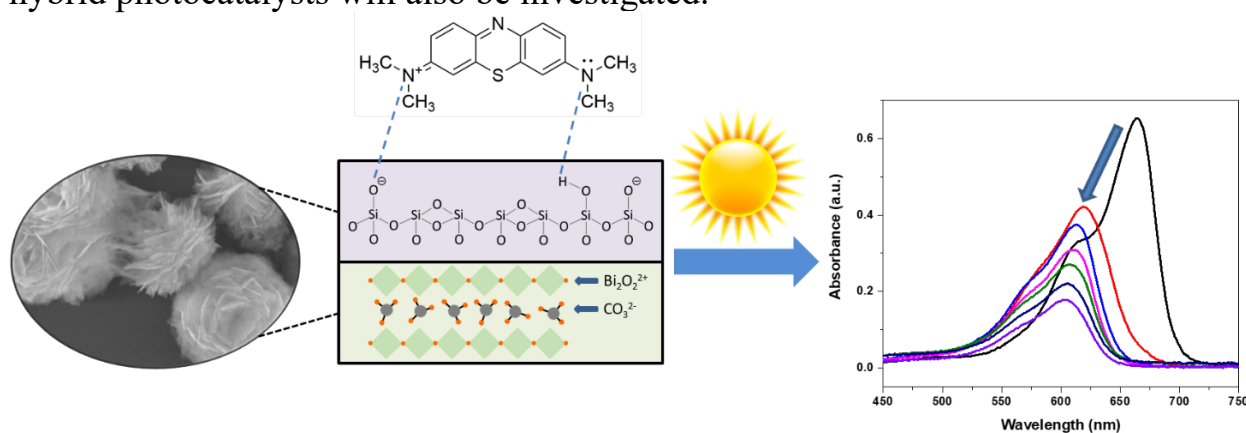


Figure: Illustration of silica-modified BSC hybrids leading to faster mineralization of methylene blue dye under sunlight.

Financial support: This project is funded by the Department of Chemical Engineering, NTNU, Trondheim.

NO₂ a Product & a Catalyst Inhibitor for Oxidation of NO at Industrial Nitric Acid Production Conditions

PhD Candidate: Jithin Gopakumar

Supervisor: Prof. Magnus Rønning

Co-Supervisors: Bjørn Christian Enger & David Waller

Nitric acid (HNO₃) is an important chemical building block and is produced industrially by the Ostwald process involving ammonia oxidation by atmospheric oxygen using Pt-Rh gauze catalysts to yield nitric oxide. The typical NO concentration at the exit of the ammonia combustor is 10%, and nitric oxide is further oxidised in a homogeneous gas phase reaction to NO₂, which is further absorbed in water to yield nitric acid. Using a catalyst to oxidise NO to NO₂ is attractive to reduce the CAPEX by replacing the bulky homogeneous oxidation process by a much more compact heterogeneously catalysed process. There is hardly any literature report on catalytic NO oxidation at high concentrations.

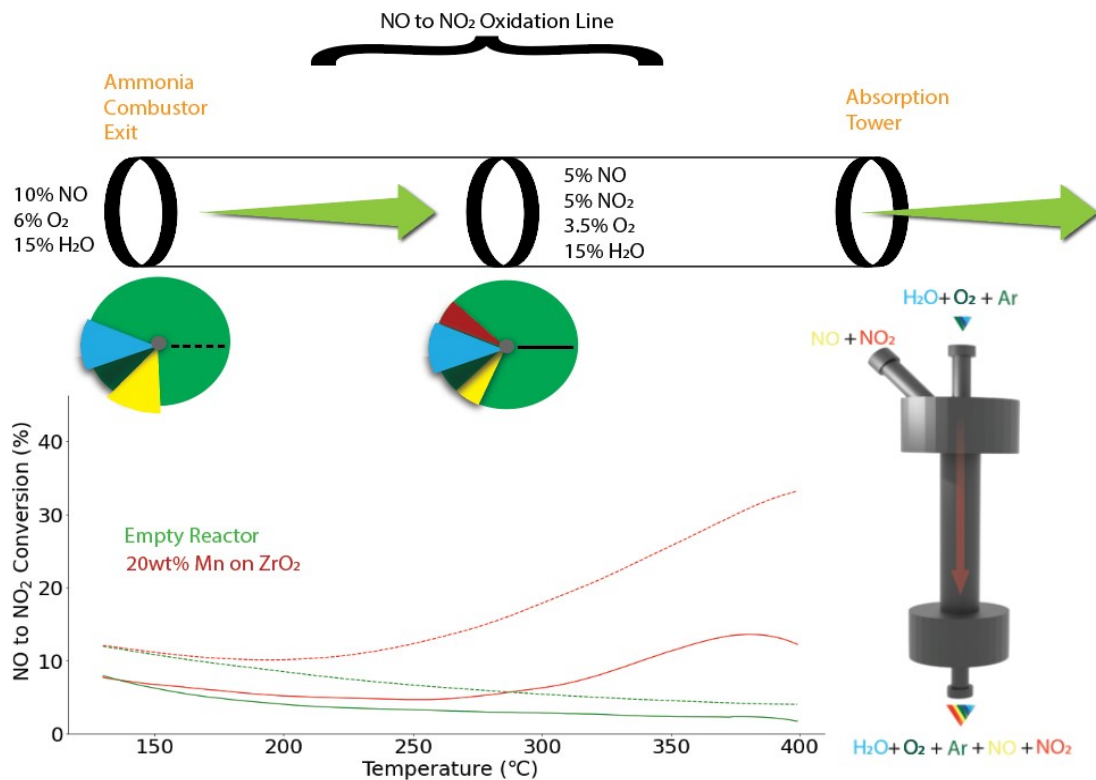


Figure: NO to NO₂ Conversion with Different Feed Compositions

However, catalytic oxidation of NO has been studied extensively in diesel engine exhaust treatment, where the NO concentration in the feed is normally in the range of 10-1000 ppm, which is very far from nitric acid production conditions. The investigated catalysts in literature so far ranges from noble metals via supported metal oxides, to ion exchanged zeolites and activated carbon fibres. The thermodynamics of the reaction itself asks for a low-temperature condition and catalytic activity is usually favoured by higher temperature. Additionally, the high concentration of nitric oxide, gas-phase conversion and the presence of water in the feed are the main challenges that hold back this reaction from being catalytic. Hence, to this date, no catalyst has been found that fully oxidises nitric oxide to nitrogen dioxide at industrial conditions.

Typical gas composition at the exit of the ammonia combustor mainly contains 10% NO, 6% O₂ and 15% H₂O. But as we move away from the ammonia combustor exit towards the absorption tower the gas composition changes to have more % of NO₂ in the feed. Hence, any novel catalyst used at this stage in nitric acid plant for NO oxidation should be able to with stand NO₂ and also be inert towards the product.

Manganese is quite widely known to be an excellent low temperature oxidation catalyst. A 20wt% Manganese on Zirconia support was prepared using incipient wetness impregnation. The current work aims to investigate NO₂ inhibition on a manganese zirconia catalyst for oxidising NO at two operating conditions, (i) 10% NO, 6% O₂ and 15%H₂O and (ii) 5% NO, 5% NO₂, 3.5% O₂ and 15%H₂O in a packed bed reactor at a space velocity of 24,000 Ncm³/h · g_{catalyst}. A temperature ramp was performed from 120-400°C. Figure 1 presents the conversion results and a clear inhibition of catalyst performance by NO₂. Moreover, the catalyst tend to reach equilibrium faster in 350-400°C temperature range with 5% NO, 5% NO₂, 3.5% O₂ and 15%H₂O as feed in comparison to 10% NO feed.

The experimental results gives further insights to an ideal location for the catalyst bed by comparing the differences in total conversions by manganese on zirconia catalyst. The favourable region for catalyst bed operation would be closer to the exit of ammonia combustor with less or no amount of NO₂ for a manganese based catalyst.

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

Kinetic studies of aqueous phase reforming

PhD Candidate: Monica Pazos Urrea

Supervisor: Prof. Magnus Rønning

Co-Supervisors: Prof. De Chen, Dr Kumar Ranjan Rout

BIKE (BImetallic catalysts **K**nowledge-based development for **E**nergy applications) is an MSCA-ITN project involving 17 European partners. Addressing to evaluate, exploit and validate the application of bimetallic catalysts in hydrogen production processes: steam reforming of biogas, aqueous phase reforming renewable feedstock, and anion exchange membrane water electrolysis.

At NTNU, we will focus our research on aqueous phase reforming (APR), a reaction carried out at low temperatures (200-300°C) and pressurized water to convert low value mixed polyols to H₂ and CO₂. The high functionality of the biomass used as a feedstock leads to the formation of non-desired products that reduce the overall yield and affect the catalyst stability [1]. Bi-metallics catalysts can achieve higher hydrogen yield and improve catalyst's thermal stability by enhancing the electronic properties and dispersion of the active metal on the support [2]. Adding Ni or Mn to

a platinum-based catalyst increases the turnover frequency of H₂ production, maintaining a high H₂ selectivity [3].

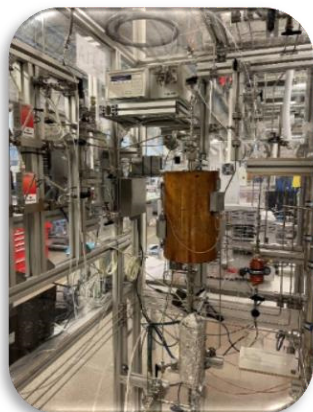


Figure. Left: experimental setup. Right: Logo of the BIKE MSCA-ITN project

In this project, we evaluate the performance of bimetallic catalysts: activity, selectivity, and stability from biomass-derived oxygenate in aqueous phase reforming, including kinetic and deactivation studies at different process conditions. In addition, we will study systems containing Pt-Ni and Pt-Mn supported in carbon materials due to their hydrothermal stability and tuneable chemical and surface properties, aiming to develop innovative bimetallic catalysts for hydrogen production.

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Financial Support: This project has received funding from the European Union’s Horizon 2020 Research and Innovation program under the Marie Skłodowska Curie Action – International Training Network (MSCA-ITN), grant agreement 813748.

Catalysts for NO_x-reduction in maritime transportation

Ph.D. Candidate: Ole Håvik Bjørkedal

Supervisor: Magnus Rønning

Co-supervisor: Rune Lødeng

Stricter regulations for maritime nitrogen oxide (NO_x) emissions are expected to create a demand for non-toxic NO_x-reduction catalysts able to perform at a wide range of operating conditions with special regards to oxygen content and temperature in the exhaust stream. Liquefied Natural Gas (LNG) is becoming more attractive as maritime fuel, due to its increasing supply and opportunity for more efficient and cleaner combustion. However, the combustion process is usually performed with surplus oxygen to minimize the risk of methane slip. Such conditions facilitate generation of thermal NO_x, 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, particularly when feeding steam to the reactor. It was suspected that H₂O was saturating the surface of the catalysts, as the deactivation was found to be reversible when steam was removed from the feed. Zirconia-supported Fe and Cu catalysts were synthesized by the same method to obtain catalysts with similar properties as the alumina-supported samples with another support. While steam still seems to be an inhibiting factor compared to “dry” feed streams, the deactivation by H₂O was not as drastic for the zirconia-based catalysts. Bimetallic Cu-Fe/ZrO₂ catalysts have shown that it is possible to draw advantage of the good low-temperature activity of Cu and higher temperature activity of Fe by combining the sites on the support, thus obtaining a wider temperature window of high activity.

The results for Cu/ZrO₂ have been published in *Catalysis Today*, while articles for Fe & Fe-Cu/ZrO₂ are in progress.

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

Advanced *in situ* and *operando* characterization of heterogeneous catalysts for sustainable process industries

PhD-candidate: Samuel K. Regli

Supervisor: Prof. Dr. Magnus Rønning

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

This PhD project is part of the industrial Catalysis Science and Innovation (iCSI) Centre. We are investigating heterogeneous catalysts during operation at industrially relevant conditions and develop the necessary data analysis tools for a multimodal data reduction and analysis to make full use of the experimental capabilities in order to link structural properties of the material with catalytic activity during reaction. We have synergies with four out of the six work packages within iCSI and collaborations within the Catalysis Group (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 the SUNCAT Group at Stanford University (Hydrogenation of CO and CO₂ to Methanol).

We 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 (XAS) with synchrotron radiation, X-ray diffraction (XRD), UV-Vis spectroscopy, Fourier-transform infrared spectroscopy (FTIR) 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 for sustainable process industry.

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.

Publications:

Bjørkedal, Ole Håvik; Regli, Samuel K.; Nuguid, Rob Jeremiah G.; Vullum, Per Erik; Kröcher, Oliver; Ferri, Davide; Rønning, Magnus. (2022) One-pot synthesis of highly dispersed mesoporous Cu/ZrO₂ catalysts for NH₃-SCR. *Catalysis Today*. vol. 384-386.

Duyar, Melis S.; Gallo, Alessandro; Regli, Samuel K.; Snider, Jonathan L.; Singh, Joseph A.; Valle, Eduardo; McEnaney, Joshua; Bent, Stacey F.; Rønning, Magnus; Jaramillo, Thomas F. (2021) Understanding Selectivity in CO₂ Hydrogenation to Methanol for MoP Nanoparticle Catalysts Using In Situ Techniques. *Catalysts*. vol. 11(1) (143).

Ma, Hongfei; Gopakumar, Jithin; Zhang, Wei; Regli, Samuel K.; Wang, Yalan; Rout, Kumar Ranjan; Fuglerud, Terje; Piccinini, Marco; Rønning, Magnus; Chen, De. (2021) Insights of the Dynamic Copper Active Sites in Ethylene Oxychlorination Studied by the Multivariate UV–vis–NIR Resolution Kinetic Approach. *Industrial & Engineering Chemistry Research*. vol. 60 (26).

Niu, Juntian; Wang, Yalan; Liland, Shirley Elisabeth Sjø; Regli, Samuel K.; Yang, Jia; Rout, Kumar Ranjan; Luo, Jun; Rønning, Magnus; Ran, Jingyu; Chen, De. (2021) Unraveling Enhanced Activity, Selectivity, and Coke Resistance of Pt–Ni Bimetallic Clusters in Dry Reforming. *ACS Catalysis*. vol. 11 (4).

Cobalt Catalyzed Fischer-Tropsch-Synthesis: Systematic Studies on Carbon Support Effects on Catalyst Activity and Deactivation

Researcher: Felix Herold

Supervisor: Prof. Dr. Magnus Rønning

One of the most fundamental problems of Cobalt based catalysts for Fischer-Tropsch synthesis (FTS) is their rapid deactivation, owing to re-oxidation of Co⁰ and sintering of Co nanoparticles. In terms of deactivation-resistant Co catalysts, the catalyst support is a key component: In addition to increasing the active Co surface area by dispersion, it promotes reducibility while stabilizing the active nanoparticles against deactivation by sintering. In this context, carbon represents an attractive support, as carbon materials are characterized by high surface areas, chemical inertness, and almost unlimited possibilities for the targeted manipulation of structure and surface chemistry. However, due to the large number of influencing factors, the impact of individual support properties (e. g. crystallinity, texture, surface chemistry) on catalytic performance and deactivation behavior of Co based FTS catalysts remains opaque. Against this background, we work on a systematic approach to disentangle carbon support effects on catalyst performance and catalyst deactivation. In this context, the influence of carbon structure, surface oxides, and heteroatom doping is studied in isolation and without interference from Co particle size effects by

combining colloidal synthesis approaches of Co nanoparticles with carefully engineered carbon supports.

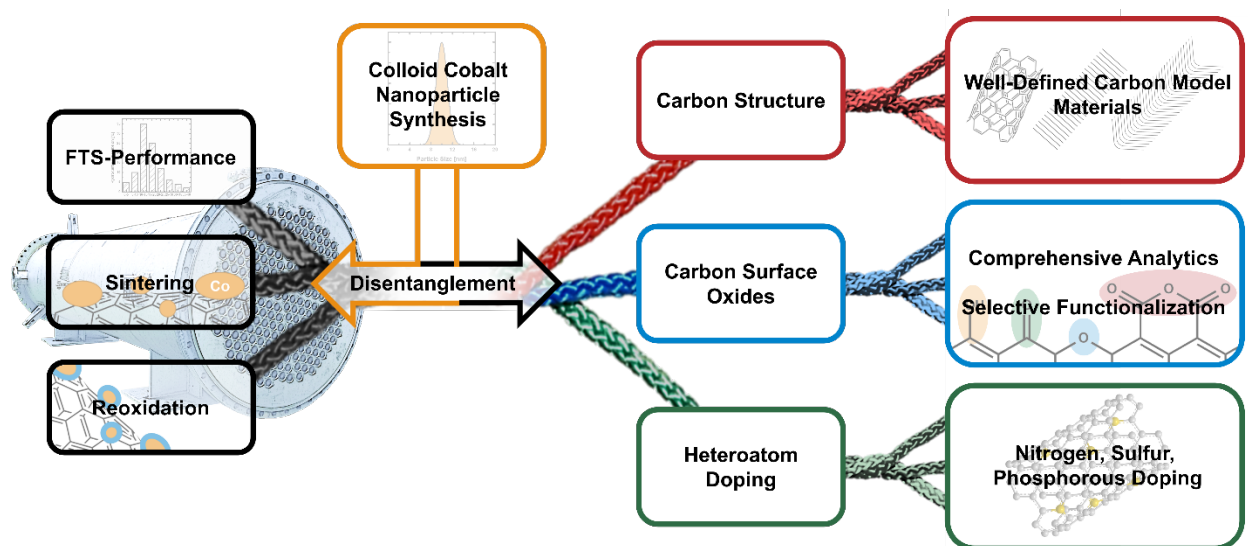


Figure: Schematic overview of colloid Cobalt NP synthesis on carbon support

Design of low-cost and carbon-resistant Ni-based mesoporous silicas for chemical CO₂ utilization through tri-reforming of methane

Postdoc: Dr. Katarzyna Świrk

Supervisor: Professor Magnus Rønning

The EU-funded Marie Skłodowska-Curie Individual Fellowship, MesoSi-CO₂ project, aims to design novel nickel-based catalysts supported on mesoporous silica. This research targets at developing an efficient synthesis route for low-cost and carbon-resistant catalysts by taking advantage of renewable bio-sources, zero-cost waste, and microwave technology. The physicochemical properties are studied by a variety of in-house characterization methods. Operando XAS-XRD (beamtime at the ESRF) results will be correlated with HRTEM to examine the nature of the nickel active phases present on the mesoporous silica. The research work is performed in collaboration with Sorbonne Université in Paris, France.

Publications in 2021:

1. Chao Sun, Katarzyna Świrk, Ye Wang, Li Li, Marco Fabbiani, Vasile Hulea, Magnus Rønning, Changwei Hu, Patrick Da Costa, Unraveling catalytic

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- properties by yttrium promotion on mesoporous SBA-16 supported nickel catalysts towards CO₂ methanation, *Fuel* (2021) article in press, doi:10.1016/j.fuel.2021.122829
- Paulina Summa, Katarzyna Świrk, Dominik Wierzbicki, Monika Motak, Ivo Alxneit, Magnus Rønning, Patrick Da Costa, Co-precipitated Ni-Mg-Al hydrotalcite-derived catalyst promoted with vanadium for CO₂ methanation, *Molecules*, 26 (2021) 6506 doi:10.3390/molecules26216506
 - Paulina Summa, Katarzyna Świrk, Ye Wang, Bogdan Samojeden, Magnus Rønning, Changwei Hu, Monika Motak, Patrick Da Costa, Effect of cobalt promotion on hydrotalcite-derived nickel catalysts for CO₂ methanation, *Applied Materials Today*, 22 (2021) 101211 doi:10.1016/j.apmt.2021.101211
 - Chao Sun, Katarzyna Świrk, Ye Wang, Katharina Sarah Scheidl, Dag Werner Breiby, Magnus Rønning, Changwei Hu, Patrick Da Costa, Tailoring the yttrium content in Ni-Ce-Y/SBA-15 mesoporous silicas for CO₂ methanation, *Catalysis Today*, 382 (2021) 104 doi:10.1016/j.cattod.2021.07.031
 - Katarzyna Świrk, Paulina Summa, Dominik Wierzbicki, Monika Motak, Patrick Da Costa, Vanadium promoted Ni(Mg,Al)O hydrotalcite-derived catalysts for CO₂ methanation, *International Journal of Hydrogen Energy*, 46 (2021) 17776, doi:10.1016/j.ijhydene.2021.02.1721
 - Chao Sun, Katarzyna Świrk, Dominik Wierzbicki, Monika Motak, Teresa Grzybek, Patrick Da Costa, On the effect of yttrium promotion on Ni-layered double hydroxides-derived catalysts for hydrogenation of CO₂ to methane, *International Journal of Hydrogen Energy*, 46 (2021), 12169, doi:10.1016/j.ijhydene.2020.03.202
 - Katarzyna Świrk, Gérard Delahay, Abdelali Zaki, Karim Adil, Amandine Cadiau, Investigation of Mn promotion on HKUST-1 metal-organic frameworks for low-temperature selective catalytic reduction of NO with NH₃, *ChemCatChem*, 13 (2021) 4029, doi:10.1002/cctc.202100431
 - Katarzyna Świrk, Gérard Delahay, Abdelali Zaki, Karim Adil, Amandine Cadiau, Facile modifications of HKUST-1 by V, Nb and Mn for low-temperature selective catalytic reduction of nitrogen oxides by NH₃, *Catalysis Today*, article in press, doi:10.1016/j.cattod.2021.07.017
 - Katarzyna Świrk, Hailong Zhang, Shanshan Li, Yaoqiang Chen, Magnus Rønning, Monika Motak, Teresa Grzybek, Patrick Da Costa, Carbon-resistant NiO-Y₂O₃-nanostructured catalysts derived from double-layered hydroxides for dry reforming of methane, *Catalysis Today*, 366 (2021) 103, doi:10.1016/j.cattod.2020.03.032

-
10. Katarzyna Świrk, Ye Wang, Changwei Hu, Li Li, Patrick Da Costa, Gerard Delahay, Novel preparation of Cu and Fe zirconia supported catalysts for selective catalytic reduction of NO with NH₃, *Catalysts*, 9 (2021) 55, doi:10.3390/catal9010056

Beamtime:

European Synchrotron Radiation Facility in Grenoble, France (05/06/2021 - 10/06/2021), XAS-XRD measurements performed within two topics:

1. MnO₂-ZrO₂ catalysts for catalytic oxidation of NO at nitric acid plant conditions
2. Operando XAS-XRD studies of Y-promoted Ni/KIT-6 catalysts for dry reforming of methane

Financial funding: The project has received funding from the European Union's Horizon 2020 research and innovation program under the Marie Skłodowska-Curie grant agreement No 892571

Advanced characterization of Pd-based membrane model systems

Project manager: Professor Hilde J. Venvik,

Project scientists: Dr. Ingeborg-Helene Svenum (SINTEF), Dr. Thijs Peters (SINTEF), Dr. Marie Døvre Strømsheim (postdoc), Senior lecturer Dr. Jan Knudsen (Lund University)

This research is part of H₂MemX, a joint effort between NTNU and SINTEF, and in cooperation with Lund University/the MAX IV Laboratory. The goal is to increase the understanding of Pd-based membranes for hydrogen separation from gas mixtures. Further knowledge of these membranes is desirable because of their role in enabling the procurement of high purity hydrogen regardless of the feedstock (biomass, natural gas). We target the investigation of the surface chemistry and segregation phenomena of the Pd-alloy membranes and model systems (i.e. single crystals), under as close as possible application conditions, by advanced surface characterization. The overall aim is to apply this knowledge towards tuning membrane performance and stability. The investigated Pd alloy membranes are manufactured by SINTEF through a two-step sputtering method that allows control of the composition and thickness.

Pd is normally alloyed with Ag, Au or Cu to enhance performance and simultaneously reduce the cost. But the introduction of a secondary metal necessitates insight into segregation phenomena as impacted by changes in exposure composition as well as conditions (T,P). The use of near ambient X-ray photoelectron spectroscopy (NAP-XPS) at the HIPPIE beamline at the MAX IV laboratory in Lund, Sweden, has allowed for in situ investigation of Pd-alloy model surfaces (single crystals) under gas exposure. CO oxidation was used as a model reaction to study the segregation behavior and surface chemistry during reaction at 1-2 mbar total pressure.

Repeated temperature ramp cycles of CO oxidation (30-600°C/150-450°C, O₂:CO=10), over Pd₇₅Ag₂₅(100) and Pd₇₅Ag₂₅(111) surfaces was performed whilst monitoring the Pd 3d and Ag 3d core levels. The results were compared to the corresponding pure Pd surfaces. The results show that the relative amount of surface Pd decreases upon heating as the inhibiting CO coverage is lifted. Although segregation was observed even at 30°C, the degree of reversibility in the segregation behavior is dependent on the experimental protocol. A protocol enabling better consistency over several temperature cycles was therefore established for the Pd₇₅Ag₂₅(111) vs Pd(111) case, and the large difference in activity between the two surfaces despite presence of surface Pd in the former points to the catalytic significance of the Pd₅O₄ surface oxide.

Acknowledgment:

This project is funded by the Research Council of Norway, project number 280903 (H2MemX – Enabling ultrathin Pd based membranes through surface chemistry diagnostics and control). Our collaborators in Lund, Virginia Boix and Dr. Jan Knudsen, acknowledge financial support from the Swedish Research Council (grant number 2017-04840). We acknowledge MAX IV Laboratory for time on Beamline HIPPIE under Proposal 20180307, 20190540 and 20190949. Research conducted at MAX IV, a Swedish national user facility, is supported by the Swedish Research council under contract 2018-07152, the Swedish Governmental Agency for Innovation Systems under contract 2018-04969, and Formas under contract 2019-02496. We gratefully acknowledge the assistance of MAX IV Laboratory staff, in particularly Dr. Andrey Shavorskiy and Dr. Suyun Zhu of the HIPPIE beamline.

Publications:

Marie D. Strømsheim, Ingeborg-Helene Svenum, Mehdi Mahmoodinia, Virginia Boix, Jan Knudsen, Hilde J. Venvik. Segregation dynamics of a Pd-Ag surface during CO oxidation investigated by NAP-XPS. *Catalysis Today* 384 (2022) 265-273.

SINTEF projects

Hydrotreating

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

The project aims to improve the performance of the client's commercial hydrotreating units. New 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)

Staff SINTEF (WP3, co-HT and co-HDO, Repsol in lead): Senior Scientist Rune Lødeng, Research Scientist Håkon Bergem, Senior Engineer Camilla Otterlei, 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.

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

Publications

[1] 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.

[2] Rune Lødeng, Håkon Bergem, Camilla Otterlei, Shirley E. Liland, Silje Fosse Håkonsen, Roman Tschentscher, *Catalytic co-refining of pyrolysis oils in rapeseed oil and straight run gas oil*, Submitted to special issue on co-refining in Energy&Fuels, December 2021

Refinery operations / Octane processes

Staff: Research scientist Hilde Bjørkan and Senior engineer Camilla Otterlei

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

Client: Equinor ASA

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

Staff SINTEF (WP4, co-HT and co-HDO, OMV lead): Senior Scientist Rune Lødeng, Research Scientist Håkon Bergem, Research Scientist Rune Myrstad, Research Scientist Nikolaos Tsakoumis, Senior Engineer Camilla Otterlei and Senior Scientist Roman Tschentscher, Senior Scientist Anette Mathiesen

Waste2Road (W2R) will develop new generation cost-effective biofuels from low cost and abundant biogenic residues and waste fractions. This will be achieved through optimization of European waste recycling logistics and development of efficient conversion technologies, giving carbon yields > 45% with greenhouse gas (GHG) savings > 80%. The consortium will deploy risk-mitigation pathways to realise industrial implementation, with primary processing at European waste recycling sites and co-processing within European refineries. SINTEF will study catalytic hydrotreating and co-hydrotreating (co-HDO) of waste cooking oils, pyrolysis oils and hydrothermal liquefaction oils from different resources at laboratory and semi-pilot scale with full pellet catalysts. Mixtures of straight run gas oil and different levels and types of renewable oils (co-HT) will also be investigated. 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.

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 (Process Technology)

Philosophiae Doctor (PhD) defenses in 2021

Defense of Jianyu Ma – Tuesday, January 26 2021

Thesis title: High temperature desulfurization of biomass-derived synthesis gas using solid sorbents

Public trial lecture on: Status and outlook for high temperature solid sorbents based CO₂ capture processes

Supervisors

Professor Edd A. Blekkan, supervisor

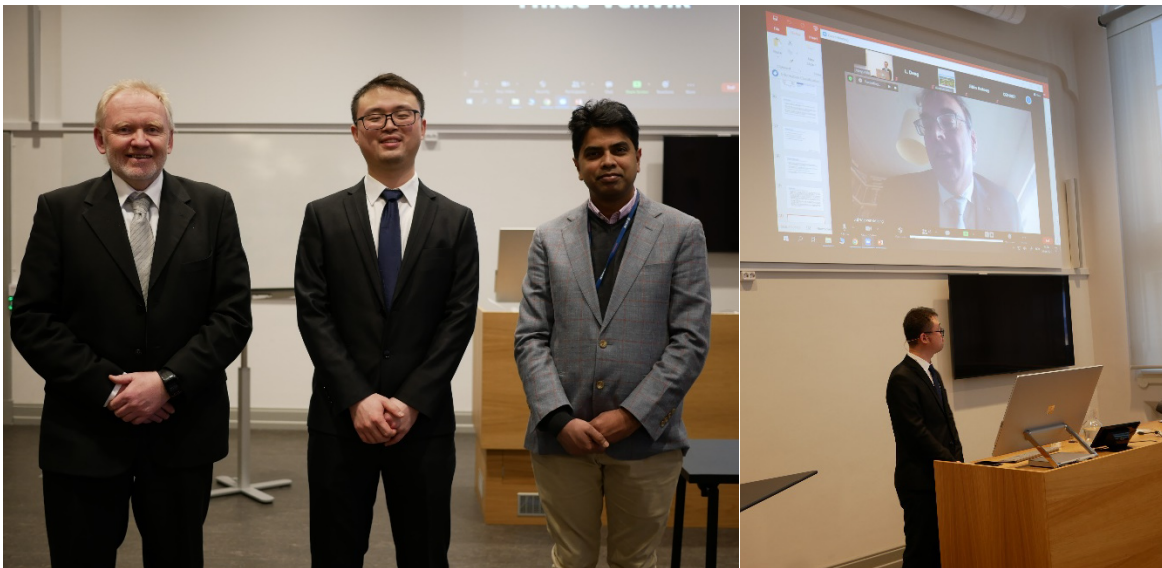
Associate Professor II Kumar Ranjan Rout, co-supervisor

Assessment Committee

Professor Wibren de Jong, TU Delft. The Netherlands

Dr. Richard Blom, SINTEF Industry, Oslo

Professor Liyuan Deng, Dept. Chem. Eng., NTNU (Administrator)



E.A. Blekkan, Jianyu Ma, Kumar R. Rout

Janyu Ma, W. de Jong

Defense of Endre Fenes – Wednesday March 17 2021

Thesis title: Ethylene oxychlorination on CuCl_2 based catalysts: Mechanism and Kinetics

Public trial lecture: Fixed bed vs fluidized bed reactors for highly exothermal reactions: pros and cons

Supervisors

Professor De Chen, supervisor

Associate Professor II Kumar Ranjan Rout, co-supervisor

Assessment Committee

Professor Dmitry Yu. Murzin, Åbo Akademi University, Finland

Professor Alessandra Beretta, Politecnico di Milano, Italy

Professor Kristin Syverud, Dept. Chem. Eng., NTNU (Administrator)



D. Chen, E. Fenes, K. Syverud, Kumar R. Rout.

D. Murzin, A. Beretta

Defense of Mohammad Zubair – Thursday March 18

Thesis title: Enhanced visible light adsorption TiO₂ based catalysts for photocatalytic H₂ generation.

Public trial lecture on: Status and perspective of ammonia as an energy carrier and the role of heterogeneous catalysts

Supervisors

Associate professor Jia Yang, supervisor

Professor Magne Rønning, co-supervisor

Assessment Committee

Professor Izumi Kumakiri, Yamaguchi University, Japan

Professor Kaiying Wang, University of South-Eastern Norway

Dr. Li He, Dept. Chem. Eng., NTNU (Administrator)



Li He, M. Zubair J. Yang

Defense of Hongfei Ma -Tuesday March 23

Thesis title: Kinetic studies of ethylene oxychlorination to ethylene dichloride and vinyl chloride.

Public trial lecture on: Catalysts in e-hydrogen and ammonia.

Supervisors

Professor De Chen, supervisor

Associate professor II Kumar Ranjan Rout-co-supervisor

Assessment Committee

Professor Tapio Salmi, Åbo Akademi University, Finland

Professor Xiang Feng, China University of Petroleum (Huadong), China

Dr. Li He, Dept. Chem. Eng., NTNU (Administrator)



Left: D. Chen, Li He, Hongfei Ma, Kumar R. Rout, top right: T. Salmi, X.Feng,
bottom right: Hongfei Ma, H. J. Venvik

Stine Lervold – Wednesday June 9

Thesis title: Investigations of the methanol to formaldehyde (MTF) reaction over silver.

Public trial lecture on: Recent developments in catalyst properties and stability for the methanation of CO₂.

Supervisors

Professor Hilde J. Venvik, supervisor

Associate professor Jia Yang, co-supervisor

Assessment Committee

Professor Leon Lefferts, University of Twente, The Netherlands.

Professor Hanna Härelind, Chalmers University of Technology, Sweden

Professor Jens-Petter Andreassen, Dept. Chem. Eng., NTNU (Administrator)



Y. Yang, S. Lervold, H. J. Venvik

Master (Diploma) Students in 2021

Vilde Roland Svensen: *The effect of metal promoters on supported cobalt catalysts for the Fischer-Tropsch Synthesis*

Albert Miró i Rovira: *Photocatalytic ammonia synthesis*

Sunniva Vold: *Efficient catalysts for attaining NO/NO₂ equilibrium in nitric acid production*

Erlend Skjørstad Værnes: *Low temperature selective hydrogenation using noble metal catalysts.*

Sunniva Skogheim: *Catalytic methane abatement for natural gas engines.*

Lasse Svendsen Chrobak: *Carbon formation and catalysis in the conversion of methyl chloride and silicone into dimethyldichlorosilane*

Vilde Vinnes Jacobsen: *Production of olefins from waste plastics*

Ida Emilie Malde Jacobsen: *Carbon formation mechanisms on Co surfaces : A DFT study*

Kristin Øxnevad Madsen: *Catalytic Steam Reforming of Hydrocarbon impurities from Biomass Gasification*

Leo Gosbert Mboyerwa: *Catalytic conversion of linocellulocellulosic biomass to flues*

Isabel Pascual García: *Preparation and characterization of of pelletized Mn-based sulfur sorbents.*



Master (diploma) students 2022

Group meetings 2021



Location: TEAMS or Room K5 - 428/429

Schedule	Time	Presenter	Topic
January 22	14:00	Martina Cazzolaro	Catalytic hydrogenation of biomass derived oxygenates to biochemicals
January 26		Jianyu Ma	Disputas (Zoom)
February 5	14:00	Petter Tingelstad	Modelling and optimization of fast hydrolysis processes for aviation fuel production.
February 19	14:00	Nikolaos Tsakoumis	12 years at KinCat; Past, Present and Beyond
March 5	14:00	Katarzyna Swirk	Nickel and yttrium containing catalysts used in dry reforming of methane; and Scientific objectives of MesoSi-CO ₂ project.
March 17		Endre Fenes	Disputas (Zoom)
March 18		Mohammad Zubair	Disputas (Zoom)
March 23		Hongfei Ma	Disputas (Zoom)
April 9	14:00	Dumitrita Spinu	Stability of solid amine structures in CO ₂ atmosphere
April 23	14:00	Ainara Moral Larrasoana	Modified Dolomite-based pellets for high temperature post-combustion CO ₂ capture.
May 7		Patricia Kooyman University of Cape Town	Bridging the pressure gap in TEM
May 21		Xingui Zhou East China University of Science & Technology	Regulating the Adsorption Configuration on metal Catalysts for semi-Hydrogenation of Acetylene
June 4		Michael Clays University of Cape Town	Catalyst characterization using in situ magnetic measurements
June 9		Stine Lervold	Disputas (Zoom)
June 18	1400	Mehdi Mahmoodina	Understanding the Coke Formation Mechanism in the Direct Synthesis of Methyl Chlorosilanes Methodology Developments.

Location: TEAMS or Room K5 - 428/429

Schedule	Time	Presenter	Topic
September 3	14:00	Info meeting	On September 2, 1400 -1600. EFCATS Award Winners presentations with Hutchings, Dimitras Pappas, Perez-Ramirez.
Sept.16 -17		Seminar. Bortistu. Storlidalen	Separate programme
September 24	15:00	Hilde J. Venvik Cathex seminar	Methanol partial oxidation to formaldehyde over silver – new kinetic and structural insights
October 1		Postponed.	Moved to September 24 (Cathex seminar)
October 15		Magnus Rønning Cathex seminar	Combination of operando characterization techniques for studies of catalysts at industrial working conditions
October 29	14:00	Felix Herold	<i>In situ</i> DRIFTS spectroscopy of surface oxides on carbon.
November 12		Anders Holmen Jia Yang Cathex seminar	Studies of the Fischer-Tropsch process. Steady-state isotopic transient kinetic analysis on catalysts for FTS
November 26	14:00	Daniel Skodvin	Enhancement in the Capacitance of Carbon-Ionic Liquid Supercapacitors by Introducing Oxygen Functional Groups
December 10	15:00	Anja O. Sjøstad Cathex seminar	From model to real catalysts operated at relevant process conditions

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 $\frac{1}{2}$ 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

TKP4176 Process operation and safety

Responsible: Professor Edd A. Blekkan

Lecturers: Edd A. Blekkan

Semester: Fall

Level: 1st year master (4th year)

Credits: 7.5 SP

Restricted Admission: Limited to 40 students

Course Plan: Lectures (3 h/week), exercises (2 h/week), self-study (7 h/week)

Objectives:

Introduction to important principles and methods of process safety.

Prerequisites:

Background as a BSc in Chemical engineering or similar.

Contents:

The course deals with operation and safety in chemical and biological processes in industry. Process operation involves a good understanding of the characteristics of different process units, how the units are designed and built, and how the units are combined. Typical process units that will be covered include tanks, separation steps, reactors and heat exchangers. The students must analyse real accidents and undesired events, and relate these to the characteristics of the units as well as to topics and phenomena from core subjects such as mass- and energy balances, fluid flow, thermodynamics, reaction kinetics, separation science and process control. Both chemical and biological processes will be used as examples in the course. Learning methods and activities:

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

Course material:

D.A. Crowl, J.F. Louvar: Chemical Process safety, 4th Edition. Pearson, 2019.

Handouts and safety websites.

Exam: Written.

TKP4155 Reaction Kinetics and Catalysis

Responsible: Associate Professor II Kumar Ranjan Rout

Lecturers: Kumar Ranjan Rout, Katarzyna Swirk

Semester: Fall

Level: 4th year

Credits: 7.5 SP

Restricted Admission: No

Course Plan: Lectures (3 h/week), exercises (2 h/week), self-study (7 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 H₂ 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.

The course is given every second year, next time in the fall term 2023.

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 2022.

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.

The course is given every second year, next time in spring 2022

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 2021

1. Niu, Juntian; Wang, Yalan; Liland, Shirley Elisabeth Sjø; Regli, Samuel K.; Yang, Jia; Rout, Kumar Ranjan; Luo, Jun; Rønning, Magnus; Ran, Jingyu; Chen, De. Unraveling Enhanced Activity, Selectivity, and Coke Resistance of Pt–Ni Bimetallic Clusters in Dry Reforming. *ACS Catalysis* 2021 11(4) 2398-2411
2. Guo, Xiaoyang; Vanhaecke, Estelle Marie M.; Vullum, Per Erik; Ma, Jianyu; Panditha Vidana, Daham Sanjaya Gunawardana; Walmsley, John; Chen, De; Venvik, Hilde Johnsen. Effects of metal dusting relevant exposures of alloy 601 surfaces on carbon formation and oxide development. *Catalysis Today* 2021 369 48-61
3. Li, Yahao; Zang, K.; Duan, Xuezhi; Luo, Jing; Chen, De. Boost oxygen reduction reaction performance by tuning the active sites in Fe-N-P-C catalysts. *Journal of Energy Chemistry* 2021 55 572-579
4. Duyar, Melis S.; Gallo, Alessandro; Regli, Samuel K.; Snider, Jonathan L.; Singh, Joseph A.; Valle, Eduardo; McEnaney, Joshua; Bent, Stacey F.; Rønning, Magnus; Jaramillo, Thomas F. Understanding Selectivity in CO₂ Hydrogenation to Methanol for MoP Nanoparticle Catalysts Using In Situ Techniques. *Catalysts* 2021 11(1) 143-
5. Bjørkedal, Ole Håvik; Regli, Samuel K.; Nuguid, Rob Jeremiah G.; Vullum, Per Erik; Kröcher, Oliver; Ferri, Davide; Rønning, Magnus One-pot synthesis of highly dispersed mesoporous Cu/ZrO₂ catalysts for NH₃-SCR *Catalysis Today* 2021 384-38 113-121
6. Xiaoyang Guo; Per Erik Vullum; Hilde J.Venvik, Inhibition of metal dusting corrosion on Fe-based alloy by combined near surface severe plastic deformation (NS-SPD) and thermochemical treatment *Corrosion Science* 2021 190 109702
7. Lervold, Stine; Lødeng, Rune; Yang, Jia; Skjelstad, Johan; Bingen, Kristin; Venvik, Hilde Johnsen. Partial oxidation of methanol to formaldehyde in an annular reactor. *Chemical Engineering Journal* 2021 423 130 -141
8. Strømsheim, Marie Døvre; Svenum, Ingeborg-Helene; Mahmoodinia, Mehdi; Boix, Virginia; Knudsen, Jan; Venvik, Hilde Johnsen. Segregation dynamics of a Pd-Ag surface during CO oxidation investigated by NAP-XPS. *Catalysis Today* 2021 384-386 265-273
9. Ma, Hongfei; Gopakumar, Jithin; Zhang, Wei; Regli, Samuel K.; Wang, Yalan; Rout, Kumar Ranjan; Fuglerud, Terje; Piccinini, Marco; Rønning, Magnus; Chen, De. Insights of the Dynamic Copper Active Sites in Ethylene Oxychlorination Studied by the Multivariate UV–vis–NIR Resolution Kinetic Approach. *Industrial & Engineering Chemistry Research* 2021 60.(26) 9437-9447
10. Summa, Paulina; Swirk, Katarzyna; Wang, Ye; Samojuden, Bogdan; Rønning, Magnus; Hu, Changwei; Motak, Monika; Da Costa, Patrick. Effect of cobalt

promotion on hydrotalcite-derived nickel catalyst for CO₂ methanation. *Applied Materials Today* 2021 25 101211

11. Summa, Paulina; Swirk, Katarzyna; Wierzbicki, Dominik; Motak, Monika; Alxneit, Ivo; Rønning, Magnus; Da Costa, Patrick. Co-precipitated Ni-Mg-Al hydrotalcite-derived catalyst promoted with vanadium for CO₂ methanation. *Molecules* 2021 26.(21) 6506

12. Sun, Chao; Swirk, Katarzyna; Wang, Ye; Li, Li; Fabbiani, Marco; Hulea, Vasile; Rønning, Magnus; Hu, Changwei; Da Costa, Patrick. Unraveling catalytic properties by yttrium promotion on mesoporous SBA-16 supported nickel catalysts towards CO₂ methanation. *Fuel* 2021 317 122829

13. Sun, Chao; Swirk, Katarzyna; Wang, Ye; Scheidl, Katharina; Breiby, Dag Werner; Rønning, Magnus; Hu, Changwei; Da Costa, Patrick. Tailoring the yttrium content in Ni-Ce-Y/SBA-15 mesoporous silicas for CO₂ methanation. *Catalysis Today* 2021 382 104-119

14. Sørli, Guro; Azim, Muhammad Mohsin; Rønning, Magnus; Mathisen, Karina. Improved lifetime and stability of copper species in hierarchical, copper-incorporated CuSAPO-34 verified by catalytic model reactions. *Physical Chemistry, Chemical Physics - PCCP* 2021 23 16785-16794

15. Ma, Jianyu; Mahmoodinia, Mehdi; Rout, Kumar Ranjan; Blekkan, Edd A. Regenerable Sorbents for High-Temperature Desulfurization of Syngas from Biomass Gasification. *Chemie Ingenieur Technik* 2021 93.(6) 949-958

16. Ma, Jianyu; Mahmoodinia, Mehdi; Rout, Kumar Ranjan; Blekkan, Edd Anders. The Impact of Operating Parameters on the Gas-Phase Sulfur Concentration after High Temperature Sulfur Sorption on a Supported Mo-Mn Sorbent. *Reactions* 2021 2 365-373

17. Pandey, Umesh; Runningen, Anders; Gavrilovic, Ljubisa; Jørgensen, Erik Andreas; Putta, Koteswara Rao; Rout, Kumar Ranjan; Rytter, Erling; Blekkan, Edd Anders; Hillestad, Magne. Modeling Fischer–Tropsch kinetics and product distribution over a cobalt catalyst. *AIChE Journal* 2021 67.(7) e17234

18. Chen, Wenyao; Cao, J.B.; Yang, Jia; Cao, Yueqiang; Zhang, Hao; Jiang, Zheng; Zhang, Jing; Qian, Gang; Zhou, Xinggui; Chen, De; Yuan, Wei-Kang; Duan, Xuezhi. Molecular-level insights into the electronic effects in platinum-catalyzed carbon monoxide oxidation. *Nature Communications* 2021 12.(1) 6888

19. Tafjord, Joakim; Rytter, Erling; Holmen, Anders; Myrstad, Rune; Svenum, Ingeborg-Helene; Christensen, Bjørn E.; Yang, Jia. Transition-Metal Nanoparticle Catalysts Anchored on Carbon Supports via Short-Chain Alginate Linkers. *ACS Applied Nano Materials* 2021 4.(4) 3900-3910

20. Wang, Yalan; Hu, Ping; Yang, Jia; Zhu, Yi-An; Chen, De. C-H bond activation in light alkanes: A theoretical perspective. *Chemical Society Reviews* 2021 50.(7) 4299-4358

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21. Wang, Yalan; Yang, Xiaoli; Xiao, Ling; Qi, Yanying; Yang, Jia; Zhu, Yi-An; Holmen, Anders; Xiao, Wende; Chen, De. Descriptor-Based Microkinetic Modeling and Catalyst Screening for CO Hydrogenation. *ACS Catalysis* 2021 11 14545-14560
 22. Bao, Yuxiang; Ma, Hongfei; Tuo, Yongxiao; Qi, Yanying; Feng, Xiang; Yang, Chaohe; Chen, De. Research progress on catalyst for the synthesis of vinyl chloride monomer (VCM). *Huagong Jinzhan* 2021 40.(4) 2034-2047
 23. Chang, Qing-Yu; Wang, Kai-Qi; Sui, Zhi-Jun; Zhou, Xingguo; Chen, De; Yuan, Wei-Kang; Zhu, Yi-An. Rational design of single-atom-doped Ga₂O₃ catalysts for propane dehydrogenation: Breaking through volcano plot by lewis acid– Base interactions. *ACS Catalysis* 2021 11.(9) 5135-5147
 24. Chen, Chen; Tuo, Yongxiao; Lu, Qing; Lu, Han; Zhang, Shengyang; Zhou, Yan, Jun; Liu, Zhanning; Kang, Zixi; Feng, Xiang; Chen, De. Hierarchical trimetallic Co-Ni-Fe oxides derived from core-shell structured metal-organic frameworks for highly efficient oxygen evolution reaction. *Applied Catalysis B: Environmental* 2021 287 119953
 25. Chen, Wenyao; Wang, Jingnan; Zhang, Yanfang; Zhang, Jing; Duan, Xuezhi; Si, Rui; Chen, De; Qian, Gang; Zhou, Xingguo. Kinetics decoupling activity and selectivity of Pt nanocatalyst for enhanced glycerol oxidation performance. *AIChE Journal* 2021 67.(10) e17339
 26. Chen, Zhaohui; Mo, Yasi; Lin, Dong; Tuo, Yongxiao; Feng, Xiang; Liu, Yibin; Chen, Xiaobo; Chen, De; Yang, Chaohe. Engineering the efficient three-dimension hollow cubic carbon from vacuum residuum with enhanced mass transfer ability towards H₂O₂ production. *Chinese Journal of Chemical Engineering* 2021 38 98-105
 27. Dar, Hassan Jamil; Jakobsen, Hugo Atle; Rout, Kumar Ranjan; Jens, Klaus-Joachim; Chen, De. Autothermal Gas-Phase Oxidative Dehydrogenation of Ethane to Ethylene at Atmospheric Pressure. *Industrial & Engineering Chemistry Research* 2021 60.(18) 6784-6802
 28. Du, Juan; Xiao, Jin; Li, Chenyang; Qiao, Jia; Chen, De; Yang, Jianhong; Zhong, Qifan; Luo, Yingtao; Chen, Kaibin; Sun, Lizhen. The preparation of three-dimensional binder-free polyaniline/aligned carbon nanotube on flexible etched Al foil substrate as high-performance pseudocapacitive cathode for nonaqueous lithium-ion capacitor. *Journal of Energy Storage* 2021 33 102165
 29. Fan, Keke; Zhang, Qiang; Li, Jianping; Chen, Deliang; Xu, Chong-Yu. The scenario-based variations and causes of future surface soil moisture across China in the twenty-first century. *Environmental Research Letters* 2021 1634061
 30. Fu, Wenzhao; Wang, Qianhong; Chen, Wenyao; Qian, Gang; Zhang, Jing; Chen, De; Yuan, Wei-Kang; Zhou, Xingguo; Duan, Xuezhi. Engineering Ru atomic

structures toward enhanced kinetics of hydrogen generation. *Chemical Engineering Science* (CES) 2021 235 116507

31. García, R.; Gil, M.V.; Rubiera, F.; Chen, De; Pevida, C. Renewable hydrogen production from biogas by sorption enhanced steam reforming (SESR): A parametric study. *Energy* 2021 218 119491

32. Hu, Wenshuo; Selli, Tommaso; Gramigni, Federica; Fenes, Endre; Rout, Kumar Ranjan; Liu, Shaojun; Nova, Isabella; Chen, De; Gao, Xiang; Tronconi, Enrico. On the redox mechanism of low-temperature NH₃-SCR over Cu-CHA: A combined experimental and theoretical study of the reduction half cycle. *Angewandte Chemie International Edition* 2021 60.(13) 7197-7204

33. Lin, Dong; Zhang, Quande; Qin, Zhengxing; Li, Qing; Feng, Xiang; Song, Zhaoning; Cai, Zhenping; Liu, Yibin; Chen, Xiaobo; Chen, De; Mintova, Svetlana; Yang, Chaohe. Reversing Titanium Oligomer Formation towards High-Efficiency and Green Synthesis of Titanium-Containing Molecular Sieves. *Angewandte Chemie International Edition* 2021 60.(7) 3443-3448

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35. Pham, Thanh Hai; Cao, Junbo; Song, Nan; Cao, Yueqiang; Chen, Bingxu; Qian, Gang; Zhou, Xingguo; Chen, De; Duan, Xuezhi. Mechanistic aspects of facet-dependent CH₄/C₂⁺ selectivity over a χ -Fe₅C₂ Fischer-Tropsch catalyst, *Green Energy & Environment* 2021 7.(3) 449-456

36. Rodríguez, S.; Capa, A.; Garcia, R.; Chen, De; Rubiera, F.; Pevida, C.; Gil, M.V..Blends of bio-oil/biogas model compounds for high-purity H₂ production by sorption enhanced steam reforming (SESR): Experimental study and energy analysis. *Chemical Engineering Journal* 2021 432 134396

37. Shan, Yu-Ling; Zhao, Wen-Ting; Zhao, Shi-Lei; Wang, Xiu-Xin; Sun, Huai-Lu; Yu, Wen-Long; Ding, Jun-Wei; Feng, Xiang; Chen, De. Effects of alumina phases on the structure and performance of VO_x/Al₂O₃ catalysts in non-oxidative propane dehydrogenation. *Molecular Catalysis* 2021 504 111466.

38. Shang, Jingyuan; Fu, Guangbin; Cai, Zhenping; Feng, Xiang; Tuo, Yongxiao; Zhou, Xin; Yan, Hao; Peng, Chong; Jin, Xin; Liu, Yibin; Chen, Xiaobo; Yang, Chaohe; Chen, De. Regulating light olefins or aromatics production in ex-situ catalytic pyrolysis of biomass by engineering the structure of tin modified ZSM-5 catalyst. *Bioresource Technology* 2021 330 124975

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40. Tuo, Yongxiao; Meng, Ying; Chen, Chen; Lin, Dong; Feng, Xiang; Pan, Yuan; Li, Ping; Chen, De; Liu, Zhanning; Zhou, Yan; Zhang, Jun. Partial positively charged Pt in Pt/MgAl₂O₄ for enhanced dehydrogenation activity. *Applied Catalysis B: Environmental* 2021 288 119996.
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43. Yan, Hao; Shen, Qi; Sun, Yinghao; Zhao, Siming; Lu, Ruilong; Gong, Mengcong; Liu, Yibin; Zhou, Xin; Jin, Xin; Feng, Xiang; Chen, Xiaobo; Chen, De; Yang, Chaohe. Tailoring Facets of α -Mn₂O₃ Microcrystalline Catalysts for Enhanced Selective Oxidation of Glycerol to Glycolic Acid. *ACS Catalysis* 2021 1.(11)6371-6383
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- Mesoporogen-Free Strategy to Construct Hierarchical TS-1 in a Highly-Concentrated System for Gas-Phase Propene Epoxidation with H₂ and O₂. *ACS Applied Materials & Interfaces* 2021 13.(22) 26134-26142
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58. Ali, Daniel; Li, Zhihui; Azim, Muhammad Mohsin; Lein, Hilde Lea; Mathisen, Karina. Evaluating pore characteristics and acid site locations in hierarchical SAPO-11 by catalytic model reactions. *Microporous and Mesoporous Materials* 2021 329 111550
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Presentations in 2021

1. Spinu, Dumitrita; Chen, De; Rout, Kumar Ranjan. (2021) Design of Low-Temperature CO₂ Adsorbents for Post-Combustion NGCC power plants: a trade-off between adsorbents' CO₂ capacity and stability. PCCC-6. UKCCS; 2021-10-19 - 2021-10-21.
2. Spinu, Dumitrita; Chen, De; Rout, Kumar Ranjan. (2021) Millimetre Scale Mesoporous Silica Spheres Impregnated with LMW PEI for the Post-combustion NGCC CO₂ Capture System. ISCRE26 & APCRE9. IIT Delhi; New Delhi. 2021-12-05 - 2021-12-08.
3. Trondheim CCS conference (TCCS-11) with an oral presentation entitled (Virtual, Trondheim): "Modified Dolomite-based pellets for high temperature post-combustion CO₂ capture, Ainara Moral, Anne Charlotte Wold, Kumar Ranjan Rout, De Chen
4. Ainara Moral, Anne Charlotte Wold, Kumar Ranjan Rout, De Chen IEAGHG 6th Post Combustion Capture Conference 19th -21st October 2021 with poster presentation entitled (Virtual, United Kingdom)
5. Ask Lysne, Kumar R. Rout, Edd A. Blekkan; Steam Reforming of Hydrocarbon Impurities from Biomass Gasification with Ni-Co/Mg(Al)O Catalysts. Bio4Fuels Days 2021, November 17-18, 2021, Drammen, Norway. Poster presentation.
6. Jibin Antony, Susana Villa Gonzalez, Sulalit Bandyopadhyay, Jia Yang, Magnus Rønning. Silica-modified bismutite nanoparticles for enhanced adsorption and visible light photocatalytic degradation of methylene blue. Contemporary solutions for advanced materials with high impact on society (CoSolMat) Workshop 2021, Bucharest, Romania, 11.10.2021-15.10.2021
7. Phuoc Hoang Ho, Katarzyna Świrk, Magdalena Jabłońska, Giancosimo Sanghez de Luna, Regina Palkovits, Gérard Delahay, Giuseppe Fornasari, Angelo Vaccari, Patricia Benito, Title: "Facile coating of Co₃O₄ on open-cell metallic foams for N₂O catalytic decomposition"XXIV International conference on Chemical Reactors ChemReactor-24, Milan, Italy–Novosibirsk, Russia, 12 - 17 September 2021, held virtually
5. Paulina Summa, Katarzyna Świrk, Ye Wang, Bogdan Samojeden, Magnus Rønning, Changwei Hu, Monika Motak, Patrick Da Costa, Effect of Co-promotion on hydrotalcite-derived Ni catalyst for CO₂ methanation, ANM 2021 in Aveiro, Portugal, 22-24July 2021, held virtually.
6. Paulina Summa, Katarzyna Świrk, Dominik Wierzbicki, Magnus Rønning, Monika Motak, Patrick Da Costa, CO₂ methanation over V-promoted hydrotalcite-derived nickel catalysts: On the effect of the catalyst preparation method, Balard Chemistry Conferences 2021 in Montpellier, France, 15-18 July 2021, held virtually andphysically.

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7. Katarzyna Świrk, Gérard Delahay, Abdelali Zaki, Karim Adil, Amandine Cadiau, Low-temperature selective catalytic reduction of NO by NH₃ over HKUST-1 catalysts impregnated with Mn Balard Chemistry Conferences 2021 in Montpellier, France, 15-18 July 2021, held virtually and physically
 8. Chao Sun, Ye Wang, Katarzyna Świrk, Magnus Rønning, Changwei Hu, Patrick Da Costa, “Monitoring the synergetic effect of yttrium and cerium of mesoporous Ce-Y/SBA-15 supported nickel catalysts for CO₂ methanation”, 15th International conference on materials chemistry (MC15), 12-15 July 2021, Royal Society of Chemistry hosted this event online
 9. Katarzyna Świrk, Chao Sun, Sandra Casale, Patrick Da Costa, Magnus Rønning, Title: “Unraveling the effect of well-dispersed nickel species in mesoporous KIT-6 for CO₂ reforming of CH₄”, Reaction kinetics, mechanisms and catalysis, 20-21 May 2021, online event from Budapest in Hungary

KinCat event at Bortistu Gjestegard, Oppdal, Norway

September 16 -17

Program Thursday September 16

08:00 – 10:45 Bus from NTNU Chemistry hall to Bortistu Gjestegard

10:45 – 11:10 *Installation in rooms and coffee & some light food*

11:10 – 13:00 Scientific presentations

11:10 – 11:20 Welcome By Edd Blekkan

11:20 – 11:40 Oscar L. I. Encinas: Conversion of synthesis gas from biomass gasification over cobalt catalyst

11:40 – 12:00 Ask Lysne: Deactivation and Coke Formation in Steam Reforming of Hydrocarbon Impurities from Biomass Gasification with Ni-Co/Mg(Al)O Catalysts

12:00 – 12:10 *Short break*

12:10 – 12:30 Kishore Rajendran: Highlights of my inevitable Ph.D. journey

12:30 – 12:50 Petter Tingelstad: Biomass to Aviation: Process design and evaluation

12:50 – 13:10 Rune Lødeng: Research activities at SINTEF – Highlights from Borealis projects

13:10 – 14:00 *Lunch*

14:00 – 17:00 Hiking or biking

19:00 - *Dinner with sauna-smoked leg of lamb from Bortistu*





Program Friday September 17

08:00 – 09:00 Breakfast

09:00 – 11:00 Scientific presentations

09:00 – 09:20 Felix Herold: The High-Temperature Acidity Paradox of Oxidized Carbon

09:20 – 09:40 Håkon Bergem: The hydrotreating project: 30 years of underground activity

09:40 – 10:00 Junbo Yu: Introduction of Pd based membrane separation technology and the challenges I met during the research

10:00 – 10:10 Short break with fruit

10:10 – 10:30 Dumitrita Spinu: Are adsorbent's high CO₂ capacity and stability enough for sorbents evaluation?

10:30 – 10:50 Ainara Moral Larrasoana: Moving Bed Carbonate-Looping (MBCL) in Post Combustion CO₂ capture

10:50 – 11:10 Jibin Antony: Silica-modified Bismutite Nanoparticles for Enhanced Adsorption and Visible Light Photocatalytic Degradation of Methylene Blue

11:10 – 13:00 Outdoor social activity

13:00 – 14:00 Lunch (in or out – depending on weather)

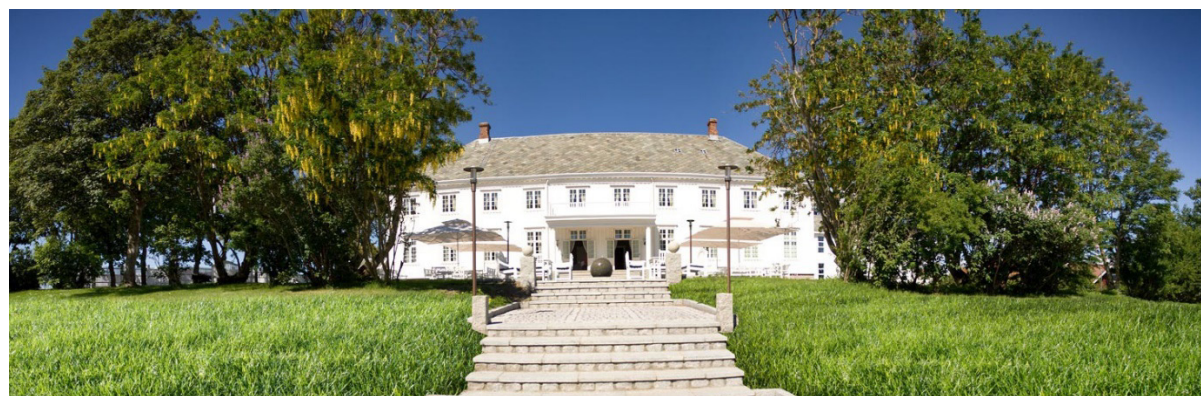
14:00 – 16:30 Bus from Bortistu Gjestegard to NTNU

Program - iCSI Annual Seminar 2021
Hovde gård, 7130 Brekstad, Norway - 18. and 19. October

Day 1 (Monday October 18)	
09:00-11:30	Registration/check-in/small talk
11:30-12:30	Lunch
12:30-13:00	Opening remarks (Chair of the Board, Pablo Beato) Status of iCSI (Director, Hilde J. Venvik)
13:00-13:30	IIA2: Silje Fosse Håkonsen & Martin Fleissner Sunding: <i>Abatement of nitrogen-containing pollutants: Characterisation studies of industrial de-N₂O catalysts</i>
13:30-14:00	IIA1: Julie Hessevik: <i>LaNiO₃ as a Pt catchment material in the ammonia oxidation process</i>
14:00-14:30	Coffee break
14:30-14:50	IIA1: Jithin Gopakumar: <i>Catalytic oxidation of NO to NO₂ for nitric acid production</i>
14:50-15:10	IIA1: Børge Holme: <i>How hard can it be to get a platinum depth profile from a palladium sample by SIMS (Secondary Ion Mass Spectrometry)?</i>
15:10-15:30	Martin Jensen, UiO: <i>Generic approach to controlled bimetallic nanoparticle synthesis</i>
15:30-15:40	IIA3: Jasmina: <i>Short summary from IIA3 activities</i>
15:40-15:50	IIA3: Youri van Valen: <i>Methanol partial oxidation to formaldehyde over silver - continued</i>
16:00-18:00	Social activity
18:15-20:00	Board meeting / Break / (IIA internal meetings or IIA6 meets the other IIAs?)
20:00-22:00	Dinner



Day 2 (Tuesday October 19)	
08:00-08:45	Breakfast
08:45-09:15	IIA6: Oleksii Ivashenko: <i>Operando APXPS studies of PtRh alloys for ammonia oxidation</i>
09:15-09:40	IIA4: Yalan Wang: <i>Promoter effects on CuCl₂/γ-Al₂O₃ catalyzed ethylene oxychlorination by DFT calculations</i>
09:40-10:00	IIA4: Wei Zhang: <i>Understanding of K , La and Mg co-promoter effect in ethylene oxychlorination by operando UV–vis-NIR spectroscopy</i>
10:00-10:30	IIA4: Kumar Rout: <i>Modelling, Estimation and Optimization of Oxychlorination of Ethylene</i>
10:30-10:50	Coffee break
10:50-11:10	IIA5: Sebastian Prodingler: <i>Synthesis-Structure-Activity Relationship in Cu-Mordenite for Partial Methane Oxidation: Directing Al Siting via Inorganic Structure Directing Agents</i>
11:10-11:20	IIA5: Bjørn Gading Solem: <i>Methylation of lower alkenes through stepwise reaction with methane</i>
11:20-11:30	IIA6: Björn Baumgarten: <i>A new ISMA – Simultaneous deactivation and deposition studies</i>
11:30-11:40	IIA6: Tina Bergh: <i>Transmission electron microscopy characterisation at NTNU</i>
11:40-12:00	IIA6: Moses Mawanga: <i>Insights into the reaction kinetics and mechanism of industrial relevant reactions</i>
12:00-13:00	Lunch
13:00-13:30	New strategies for the industry partners
13:30-13:50	Closing remarks
14:30	Departure Coastal express to Trondheim
15:40	Departure by air to Oslo from Brekstad Airport
16:05	Departure Coastal express to Trondheim



Alumni – PhD students Catalysis group

Stine Lervold

Defense of thesis: June 2021

Thesis title: *Investigation of the methanol to formaldehyde (MTF) reaction over silver.*

Trial lecture: *Recent developments in catalyst properties and stability for the methanation of CO₂*

Current position: Senior Engineer Operation & Maintenance, Equinor, Trondheim.

Hongfei Ma

Defense of thesis: March 2021

Thesis title: *Kinetic Studies of Ethylene Oxychlorination to Ethylene Dichloride and Vinyl Chloride*

Trial lecture: *Catalysts in e-hydrogen and ammonia*

Current position: Postdoctoral Fellow at KinCat, NTNU, Trondheim, Norway.

Muhammad Zubair

Defense of thesis: March 2021

Thesis title: *Enhanced visible light adsorption TiO₂ based catalysts for photocatalytic H₂ generation.*

Trial lecture: *Status and perspective of ammonia as an energy carrier and the role of heterogeneous catalysts*

Current position: Postdoctoral Research Fellow at Tampere University, Finland.

Endre Fenes

Defense of thesis: March 2021.

Thesis title: *Ethylene oxychlorination on CuCl₂ based catalysts. Mechanism and Kinetics.*

Trial lecture: *Fixed-bed vs fluidized bed reactors for highly exothermal reactions; pros and cons*

Current position: Process Engineer, ArcticNor AS, Larvik, Norway.

Jianyu Ma

Defense of thesis: January 2021

Thesis title: *High-temperature desulfurization of biomass-derived synthesis gas using solid sorbents*

Trial lecture: *Status and outlook for hightemperature solid sorbents based CO₂ capture processes*

Current position: BYD, Shenzhen, China.

Xiaoyang Guo

Defense of thesis: June 2020

Thesis title: *Inhibiting carbon growth at the initial stage of metal dusting corrosion of high temperature alloys*

Trial lecture: *Gaseous reduction of metal oxides – in particular iron oxides*

Current position: Principal Engineer, NTNU, Trondheim.

Ata ul Rauf Salman

Defense of thesis: December 2019

Thesis title: *Catalysts for attaining NO/NO₂ equilibrium*

Trial lecture: *Nitrogen fixation beyond Haber-Bosch - recent developments in heterogeneous catalysis and electrocatalysis*

Current position: Process Engineer, Equinor, Porsgrunn, Norway.

Martina Francisca Baidoo

Defense of thesis: April 2019

Thesis title: *Ethylene Oxychlorination on CuCl₂based Catalysts: Operando Kinetic Study*

Trial lecture: *Catalytic process for plastic recycling*

Current position: Lecturer, Kwame Nkrumah University of Science and Technology, Ghana.

Yalan Wang

Defense of thesis: March 2019

Thesis title: *Model-aided catalyst prediction through descriptor-based hybrid semi-empirical approach*

Trial lecture: *Machine Learning in Heterogeneous Catalysis*

Current position: Senior Engineer, Aker Solutions, Trondheim, Norway.

Isaac Yeboah

Defense of thesis: February 2019

Thesis title: *Tandem Catalytic Upgrading of Biomass. Fast-Pyrolysis Constituents to Fuels*

Trial lecture: *Progress in single atom catalysis*

Current position: Process Development Engineer at INEOS Olefins and Polymers, Spring, Texas, USA.

Erik Østbye Pedersen

Defense of thesis: June 2018

Thesis title: *Mn promotion effects in Co based Fischer-Tropsch production of light olefins*

Trial lecture: *Hydrogen production from hydrocarbons vs. water electrolysis: A comparison of capital and operation expenses as a function of electricity and hydrocarbon prices*

Current position: NAMMO, Raufoss, Norway.

Ljubisa Gavrilovic

Defense of thesis: April 2018

Thesis title: *Fischer-Tropsch synthesis – Influence of aerosol – deposited potassium salts on activity and selectivity of Co based catalysts*

Trial lecture: *A critical view on different pathways to convert biomass to chemicals and fuels*

Current position: Scientist, IFE, Kjeller, Norway.

Yahao Li

Defense of thesis: March 2018

Thesis title: *Sustainable electrocatalysts for oxygen reduction reaction. M-N-P (M: transition metals) doped mesoporous carbon from biomass.*

Trial lecture: *Synthetic fuels – polyoxymethylene dimethyl ethers as bridging technology for the diesel engine*

Current position: Postdoctoral Researcher, Zhejiang University, Hangzhou, China

Marie Døvre Strømsheim

Defense of thesis: December 2017

Thesis title: *Co₁₁₋₂₀ and Pd₃Au₁₀₀ single crystals as catalyst model system.*

Trial lecture: *Metal-Organic-Frameworks (MOFs) – Properties and applications in catalysis*

Current position: Product developer, Hydrogen Mem-Tech, Trondheim, Norway.

Ida Hjort

Defense of thesis: March 2017

Thesis title: *Catalysis for electrochemical conversion of CO₂ in aqueous solutions*

Trial lecture: *State of the art and perspectives in catalytic processes for CO₂ conversion into chemicals and fuels*

Current position: Research Scientist at SINTEF Energi AS, Trondheim.

Marthe Emelie Melandsø Buan

Defense of thesis: March 2017

Thesis title: *Nitrogen-doped Carbon Nanofibers for the Oxygen Reduction Reaction*

Trial lecture: *Photoelectrochemical CO₂ Reduction to Alcohols*
Current position: Project Engineer at ReSiTec, Kristiansand.

Xuehang Wang

Defense of thesis: September 2016

Thesis title: *Porous carbon prepared by chemical activation for high-energy supercapacitors in ionic liquid electrolyte*

Trial lecture: *Recent progress in electrochemical production and conversion of hydrogen*

Current position: Assistant Professor at Technische Universiteit Delft, The Netherlands.

Farbod Dadgar

Defense of thesis: June 2016

Thesis title: *Direct synthesis of dimethyl ether in microstructured reactors: The interactions between methanol synthesis and methanol dehydration*

Trial lecture: *Electrocatalysis for electromobility - current status, challenges and future approaches to solve the catalytic limitations in batteries*

Current position: R&D Manager, Cambi, Oslo, Norway.

Yanying Qi

Defense of thesis: April 2016

Thesis title: *Mechanistic Insights into Cobalt-based Fischer-Tropsch Synthesis*

Trial lecture: *Catalysis for synthesis gas production and utilization, beyond FTS: state-of-the-art and reaction mechanisms*

Current position: Business Data Analyst, Apear, Trondheim, Norway.

Anh Hoang Dam

Defense of thesis: December 2015

Thesis title: *Bimetallic Catalyst System for Steam Reforming*

Trial lecture: *The Principles of the Fluid Catalytic Cracking (FCC) Process – The Influence of Feedstock Quality, Reactor Technology and Operating Conditions*

Current position: Senior Material Chemist, CealTech AS, Stavanger, Norway.

Andrey Sergeevich Volynkin

Defense of thesis: September 2015

Thesis title: *The role of carbon supports in platinum catalyzed hydrogenation/dehydrogenation model reaction.*

Trial lecture: *Catalytic oxidation of methane and other hydrocarbon in dilute mixtures*

Current position: Senior Engineer, Institute of Marine Research, Bergen, Norway.

Andreas Helland Lillebø

Defense of thesis: September 2014

Thesis title: *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.*

Trial lecture: *Concepts for energy storage utilizing catalysis beyond Fischer-Tropsch synthesis*

Current position: COO, Cambi, Oslo, Norway.

Georg Voss

Defense of thesis: August 2014

Thesis title: *Mesostructured alumina and the state of Ni as promotor for Co Fischer-Tropsch synthesis catalysts.*

Trial lecture: *Concepts and challenges in catalytic waste-water treatment*

Current position: Process Development Scientist, REEtec, Porsgrunn, Norway.

Nicla Vicinanza

Defense of thesis: May 2014

Thesis title: *An investigation of fundamental phenomena affecting the performance of sputtered Pd alloy thin film membranes for hydrogen separation*

Trial lecture: *Production of medium to high purity oxygen; an evaluation of alternative methods and applications*

Current position:

Alexey Voronov

Defense of thesis: February 2014

Thesis title: *Sensitivity enhancement of X-ray absorption spectroscopy applied to Co-based Fischer-Tropsch synthesis catalysts*

Trial lecture: *Kinetic modeling of catalytic deNO_x chemistry –state of art and recent progress in methodology and mechanistic insight*

Current position: Deputy CEO i SuperOx, Russia.. Moscow, Russia.

Daham Sanjaya Gunawardana Panditha Vidana

Defense of thesis: January 2014

Thesis title: *Carbon formation phenomena and the initial stage of metal dusting corrosion - an experimental investigation*

Trial lecture: *Mixed-metal oxide catalysts for ammonia oxidation*

Current position: Yara, Porsgrunn.

Fengliu Lou

Defense of thesis: September 2013

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

Trial lecture: *Challenges in large scale chemical and electrochemical energy storage*

Current position: Beyond AS, Stavanger.

Ingvild Tronstad

Defense of thesis: June 2013

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

Trial lecture: *Thermal analysis: Principles, techniques and applications in catalyst characterization*

Current position: NAMMO Raufoss.

Tayyaba Noor

Defense of thesis: June 2013

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

Trial lecture: *Catalytic combustions: catalysts and applications*

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

Ilya Viktorovich Gorelkin

Defense of thesis: March 2013

Thesis title: *Concepts and models of the catalytic dehydrogenation of propane.*

Trial lecture: *SCR-deNO_x catalysis: Catalysis and processes for NO_x removal from mobile sources*

Current position: CTO, Naukatek, Trondheim, Norway.

Paul Radstake

Defense of thesis: December 2012

Thesis title: *Dehydrogenation of Ethane over Alumina-Supported Pt-Sn Catalysts*

Trial lecture: *Metal Nanoparticles in Catalysis*

Current position: Franzefoss Minerals, Hylla, Norway.

Eleni Patanou

Defense of thesis: September 2012

Thesis title: *Adsorption Microcalorimetry studies on Cobalt Catalysts*

Trial lecture: *Production of light olefins from syngas*

Current position: Coordinator NTNU Energy, Trondheim.

Hassan Jamil Dar

Defense of thesis: August 2012

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

Trial lecture: *Compact steam reformers*

Current position:

Navaneethan Muthuswamy

Defense of thesis: December 2011

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

Trial lecture: *Graphene, synthesis and energy related applications*

Current positions: Research Engineer at Vianode, Oslo, Norway.

Kazi Saima Sultana

Defense of thesis: November 2011.

Thesis title: *Calcium Based CO₂ Acceptors for Sorption Enhanced Steam Methane Reforming*

Trial lecture: *Catalytic conversion of CO₂*

Current position: Senior Engineer, IFE, Kjeller, Norway.

Nikolaos E. Tsakoumis

Defense of thesis: November 2011

Thesis title: *Deactivation of cobalt based Fischer-Tropsch synthesis catalysts*

Trial lecture: *Recent progress in in situ vibrational spectroscopy for catalytic applications*

Current position: Research Scientist, SINTEF, Trondheim, Norway.

Jia Yang

Defense of thesis: October 2011

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

Trial lecture: *Carbide, Nitride and mixed oxide as replacements for noble metal catalysts*

Current position: Assoc. Professor, NTNU, Trondheim, Norway.

Oana Mihai

Defense of thesis: September 2011

Thesis title: Thesis title: *Partial Oxidation of Methane by Chemical Looping*
Trial lecture: *Biomass conversion by pyrolysis and subsequent catalytic upgrading*
Current position: EATS Research Engineer, Volvo Car Group, Sweden.

Fan Huang

Defense of thesis: August 2011
Thesis title: *3D Carbon/polyaniline Nanostructures for Energy Storage*
Trial lecture: *Catalysis in energy storage*
Current position: CealTech AS, Stavanger, Norway.

Shreyas Pandurang Rane

Defense of thesis: May 2011
Thesis title: *Relation between Catalyst Properties and Selectivity in Fischer-Tropsch Synthesis*
Trial lecture: *Catalytic Cleaning of Marine Fuel Exhaust Emissions*
Current position:

Fatemeh (Fatima) Hayer

Defense of thesis: March 2011.
Thesis title: *Direct Synthesis of Dimethyl Ether in Microstructured Reactors*
Trial lecture: *Recent developments in the Fischer-Tropsch Synthesis over iron catalysts*
Current position: Principal Process Engineer, Moreld Apply, Stavanger, Norway.

Xuyen Kim Phan

Defense of thesis: January 2011
Thesis title: *Catalyst formulations for use in microstructured reactors for conversion of synthesis gas to liquids.*
Trial lecture: *Direct catalytic conversion of carbohydrates to hydrocarbons*
Current position: WellChem AS.

Hamidreza Bakhtiary

Defense of thesis: November 2010
Thesis title: *Performance assessment of a packed bed microstructured reactor – heat exchanger for methanol synthesis from syngas.*
Trial lecture: *Production of C2-C4 alcohols from synthesis gas*
Current position: Technology Licensing Manager, Dynea, Oslo, Norway

Sara Boullosa Eiras

Defense of thesis: October 2010

Thesis title: *Comparative study of selected catalysts for methane partial oxidation.*
Trial lecture: *Catalysts and materials development in solid oxide fuel cells*
Current position: Principal Engineer, Yara, Porsgrunn, Norway.

Li He

Defense of thesis: January 2010
Thesis title: *Sorption enhanced steam reforming of biomass derived compounds*
Trial lecture: *Conversion of algal-based biomass by thermochemical methods: opportunities and challenges*
Current position: Innovation manager, NTNU, Trondheim, Norway.

Astrid Lervik Mejdell

Defense of thesis: May 2009
Thesis title: *Properties and application of 1-5 μ m Pd/Ag23wt.% membranes for hydrogen separation*
Trial lecture: *Recent advances in photocatalysis*
Current position: Principal Researcher, Equinor.

Nina Hammer

Defense of thesis: November 2008
Thesis title: *Au-TiO₂ catalysts supported on carbon nanostructures for CO removal reactions*
Trial lecture: *Production of C₂ oxygenates from syngas*
Current position: Yara, Porsgrunn, Norway.

Bjørn Christian Enger

Defense of thesis: December 2008
Thesis title: *Hydrogen production by catalytic partial oxidation of methane.*
Trial lecture: *Synthesis and application of core-shell structured nanoparticles (CSNP) in catalysis*
Current position: Researcher, SINTEF, Trondheim, Norway.

Silje Fosse Håkonsen

Defense of thesis: June 2008
Thesis title: *Oxidative dehydrogenation of ethane at short contact times.*
Trial lecture: *Catalysis in high temperature fuel cells*
Current position: Researcher, SINTEF industri, Oslo, Norway.

Hilde Meland

Defense of thesis: May 2008

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

Trial lecture: *In situ/operando studies of working catalysts*

Current position: Researcher, SINTEF industri, Trondheim, Norway.

Ingvar Kvande

Defense of thesis: December 2007

Thesis title: *Carbon nanofiber supported platinum catalysts.*

The role of catalysts in metal dusting

Current position: Researcher, NORSØK, Tingvoll, Norway.

Svatopluk Chytil

Defense of thesis: September 2007

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

Trial lecture: *Synthesis and catalytic applications of mesoporous alumina*

Current position. Senior Chemical Engineer, Quantafuel, Norway.

Hilde Dyrbeck

Defense of thesis: September 2007

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

Trial lecture: *Hydrogen storage in organic hydrides*

Current position: Principal Engineer, Equinor, Trondheim, Norway.

Espen Standal Wangen

Defense of thesis: May 2007

Thesis title: *Characterisation and pyrolysis of heavy oils*

Trial lecture: *Transportation fuels from biomass*

Current position: Teacher, Charlottenlund ungdomsskole, Trondheim.

Øyvind Borg

Defense of thesis: April 2007

Thesis title: *Role of alumina support in cobalt Fischer-Tropsch synthesis.*

Trial lecture: *Challenges to catalysis in sustainable power generation from natural gas*

Current position: Senior Engineer, Equinor, Trondheim, Norway.

Florian Huber

Defense of thesis: August 2006

Thesis title: *Nanocrystalline copper-based mixed oxide catalysts for water-gas shift*
Trial lecture: *Catalysis in confined geometries – state of the art and relevance to industrial catalysis*

Current position: Head of New Technologies & Incubation, the GmbH, Germany.

Vidar Frøseth

Defense of thesis: May 2006

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

Trial lecture: *Catalytic upgrading of residues*

Current position: Equinor, Mongstad.

Erlend Bjørgum

Defense of thesis: January 2006

Thesis title: *Methane conversion over mixed metal oxides*

Trial lecture: *Photocatalysis*

Current position: Equinor, Mongstad.

Sølvi Storsæter

Defense of thesis: June 2005

Thesis title: *Fischer-Tropsch synthesis over cobalt supported cobalt catalysts.*

Trial lecture: *Removal of NO_x by catalytic processes*

Current position: Equinor, Mongstad.

Ingrid Aartun

Defense of thesis: June 2005

Thesis title: *Microstructured reactors for hydrogen production.*

Trial lecture: Non-conventional methods for producing olefins from ethane and propane

Current position: Equinor, Stavanger.

Kjersti O. Christensen

Defense of thesis: March 2005

Thesis title: *Steam reforming of methane on different nickel catalysts.*

Trial lecture: *Synthesis gas from biomass*

Current position Equinor, Trondheim.

Zhixin Yu

Defense of thesis: January 2005

Synthesis of carbon nanofibers and carbon nanotubes.

Nanocatalysis. Mature Science Revisited or Something New?

Current position: Professor, UiS, Stavanger.

Thomas Løften

Defense of thesis: December 2004

Thesis title: *Catalytic isomerisation of light alkanes*

Trial lecture: *Catalytic removal of nitrogen oxides under oxidizing conditions*

Current position: Equinor, Mongstad.

Kjetil Hauge

Defense of thesis: September 2004.

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

Trial lecture: *Non-conventional routes to petrochemicals and fuels from natural gas*

Current position: Equinor.

Christian Aaserud

Defense of thesis: May 2003.

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

Trial lecture: *Catalytic Materials for Fuel Cell Applications*

Current position: Gassco.

Bozena Silberova

Defense of thesis: January 2003

Thesis title: *Oxidative dehydrogenation of ethane and propane at short contact time*

Trial lecture: *Catalytic combustion*

Current position: Kuiper & Burger Advies- en Ingenieursbureau, Netherlands.

Petr Steiner

Defense of thesis: December 2002

Thesis title: *Kinetic and deactivation studies of hydrodesulfurization catalysts*

Trial lecture: *Transportation fuels and fuel components from biomass. Raw materials, production and performance*

Current position: AR/VR Expert, Sales Director at Avatar Media, Prague, Czechia.

Leiv Låte

Defense of thesis: 2002

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

Trial lecture: *Catalysis in supercritical fluids*
Current position: CEO at IC Technology AS, Trondheim.

Sten Viggo Lundbo

Defense of thesis: June 2002.
Thesis title: *Hydrogenation of carbon monoxide over zirconia and modified zirconia catalysts.*
Trial lecture: *Materials and processes for selective adsorption of CO₂*
Current position: Equinor, Stavanger.

Lucie Bednarova (Duesterhoeft)

Defense of thesis: May 2002
Thesis title: *Study of supported Pt-Sn catalysts for propane dehydrogenation.*
Trial lecture: *Computational Catalysis*
Current position: Senior Researcher at General Motors, Detroit, USA.

Thomas Sperle

Defense of thesis: October 2001.
Thesis title: *Steam reforming of hydrocarbons to synthesis gas.*
Trial lecture: *Nanostructured Materials in Heterogeneous Catalysis*
Current position: CTO at IC Technology, Trondheim.

Torbjørn Gjervan

Defense of thesis: November 2000
Thesis title: *Studies of bimetallic particle formation in reforming catalysts.*
Trial lecture: *Recent advanced in direct conversion of methane*
Current position: Research manager, SINTEF.

Marcus Fathi

Defense of thesis: September 2000
Thesis title: *Catalytic partial oxidation of methane to synthesis gas.*
Trial lecture: *Heterogenization of homogeneous catalysts*
Current position: Equinor, Trondheim.

Magnus Rønning

Defense of thesis: February 2000
Thesis title: *Bimetallic catalysts and platinum surfaces studied by X-ray absorption spectroscopy and scanning tunnelling microscopy*
Trial lecture: *Photocatalysis*
Current position: Professor, NTNU.

Ketil Firing Hanssen

Defense of thesis: 1999

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

Trial lecture: *The Role of Hydrogen in the Production of Hydrogen*

Current position: Principal engineer, DNV GL.

Marit Senum Brownrigg

Defense of thesis: August 1999

Thesis title: *Deactivation and regeneration of bifunctional zeolites*

Trial lecture: *In situ Production of Hydrogen for Fuel Cells in Cars*

Current position: Jotun, Sandefjord.

Hans Petter Rebo

Defense of thesis: March 1999

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

Trial lecture: *Alkylation processes based on solid catalysts*

Current position: Director Electro and Energy at Norsk Industri.

De Chen

Defense of thesis: 1998

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

Trial lecture: *Prevention of deactivation due to coke deposition. A multiscale approach*

Current position: Professor, NTNU.

Mimmi Kjetså

Defense of thesis: May 1998

Thesis title: *Etherification of methanol and iso/n-propanol with C4–C6 olefins on a macroporous acid ion exchange resin catalyst*

Trial lecture: *Methods for Controlling the Content of Aromatics in Gasoline*

Current position: Equinor, Stjørdal.

Staale Førre Jenssen

Defense of thesis: January 1998

Thesis title: *Catalytic decomposition of NO over metal exchanged zeolites*

Trial lecture: *Catalytic fixation of carbon dioxide*

Current position: Equinor, Trondheim.

Håkon Bergem

Defense of thesis: April 1997

Thesis title: *Sulfur tolerant zeolite supported platinum catalysts for aromatics hydrogenation.*

Trial lecture: *Preparation of Supported Metal Catalysts*

Current position: Senior researcher, SINTEF.

Karina Heitnes Hofstad

Defense of thesis: 1996

Thesis title: *Catalytic oxidation of methane to synthesis gas*

Trial lecture: *Chemical nitrogen fixation*

Current position: Equinor, Trondheim, Norway.

Anne-Mette Hilmen

Defense of thesis: October 1996

Thesis title: *Reduction and reoxidation of cobalt Fischer-Tropsch catalysts*

Trial lecture: *Catalysis by Solid Super Acids*

Current position: Deputy Director General at Norwegian Ministry of Petroleum and Energy, Oslo, Norway

Rune Prestvik

Defense of thesis: October 1995

Thesis title: *Characterization of the metal function of a Pt-Re/Al₂O₃ reforming catalyst.*

Trial lecture: *Upgrading of light (C₂-C₄) alkanes by catalytic processes*

Current position: Equinor. Trondheim, Norway.

Sturla Vada

Defense of thesis: October 1994

Thesis title: *Isotopic transient kinetic investigations of catalytic reactions.*

Trial lecture: *Spillover in catalysis*

Current position: Aker BP, Trondheim.

Arne Grønvold

Defense of thesis: September 1994

Thesis title: *Conversion of methanol to lower alkenes over molecular sieve-type catalysts*

Trial lecture: *Oxygenates as Fuel Components – Processes and Applications*

Current position: Inovyn, Herøya, Norway

Geir Remo Fredriksen

Defense of thesis: December 1993

Thesis title: *Hydrogenation of CO on supported cobalt catalysts studied by in situ FTIR spectroscopy*

Trial lecture: *Catalytic Combustion*

Current position: Equinor.

Odd Arne Bariås

Defense of thesis: December 1993

Thesis title: *Transient kinetic investigation of the catalytic dehydrogenation of propane*

Trial lecture: *Application of Rare Earth in Catalysis*

Current position: Elkem Solar AS

Stein Harald Skaare.

Defense of thesis: December 1993

Thesis title: *Reaction and heat transfer in wall-cooled fixed bed reactor*

Trial lecture: *The Use of Transient Techniques in Kinetic Studies.*

Current position: Aibel, Oslo

Anne Hoff

Defense of thesis: October 1993

Thesis title: *CO hydrogenation over cobalt Fischer-Tropsch catalysts.*

Trial lecture: *Production of i-butene*

Current position: Senior Advisor, Department of Chemical Engineering, NTNU, Trondheim

Ola Olsvik

Defense of thesis: 1993

Thesis title: *Thermal coupling of methane*

Trial lecture: *Catalytic membrane reactors*

Current position: Equinor.

Trude Dypvik

Defense of thesis: January 1992

Thesis title: *Oligomerization of ethene on zeolite ZSM-5 type catalysts*

Trial lecture: *Syntesegass fra metan*

Current position: Senior advisor, The Research Council of Norway.

Rune Lødeng

Defense of thesis: 1991

Title of thesis: *A kinetic model for methane directly to methanol.*

Trial lecture: *Technologies for formation of synthesis gas*

Current position: Senior researcher, SINTEF Trondheim.

Edvard Bergene

Defense of thesis: March 1990

Thesis title: *Surface characterization of Pt and Pt/Rh gauze catalysts.*

Trial lecture: *Katalytisk rensing av eksosgasser*

Current position: Equinor.

Kjell Moljord

Defense of thesis: 1986

Thesis title: *Diffusjon og reaksjon i sure organiske ionebyttere: Væskefase dehydratisering av metanol og t-butanol katalysert av sulfonert poly(styrene-divinylbenzen).*

Trial lecture: Methods for controlling the content of aromatics in gasoline.

Current position: Equinor, Adjunct professor, NTNU.

Dag Schanke

Defense of thesis: October 1986

Thesis title: *Hydrogenation of CO over supported iron catalysts.*

Trial lecture: *Katalytiske egenskaper til ikke-oksydiske keramer.*

Current position: Retired from Equinor, Trondheim.

Edd Anders Blekkan

Defense of thesis: December 1985

Thesis title: *Characterization and pyrolysis of heavy oils.*

Trial lecture: *Katalytisk hydrogenbehandling*

Current position: Professor NTNU Trondheim, Norway.

Per Åge Sørum

Hydrogenolysis of esters. Conversion of metylformiat to methanol

Defense of thesis: 1982

Current position: Retired from Statoil Mongstad