Annual Report

2020

KinCat

Catalysis Group – SINTEF – NTNU

KinCat
Strong Point Centre Kinetics and Catalysis

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

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Annual Report 2020
KINCAT
Strong Point Centre Kinetics and Catalysis

Contents

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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

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Coordinator Anne Hoff (60%)

Laboratory personnel:

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Senior Engineer Anne Hoff (10%)

Doctoral students 2020/2021:

Stine Lervold
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Daniel Skodvin
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Martina Cazzolaro
Jianyu Ma
Hongfei Ma
Mario Ernesto Casalegno
Joakim Tafjord
Jibin Antony
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Junbo Yu
Monica Pazos Urrea
Endre Fenes
Petter Tingelstad
Youri van Valen
Oscar Ivanez Encinas
Jithin Gopakumar
Kishore Rajendran
Wei Zhang

Postdoctoral fellows/Researchers 2020/2021

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

Visitors 2020/2021

Consolato Rosmini
Javier Torres (Aug – Dec 2020)

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

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

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Senior Scientist Bjørn Christian Enger
Senior Scientist Rune Lødeng
Research Scientist Rune Myrstad
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Senior Engineer Camilla Otterlei

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Kjell Moljord


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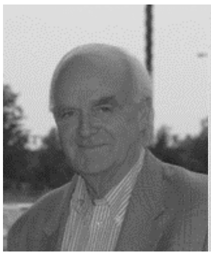
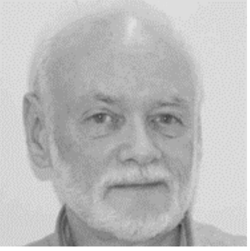
Ingeborg-Helene Svenum


Anders Holmen


Erling Rytter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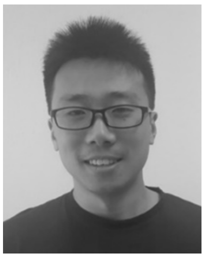
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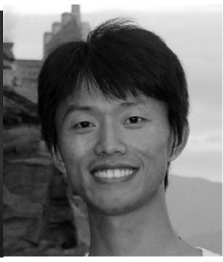
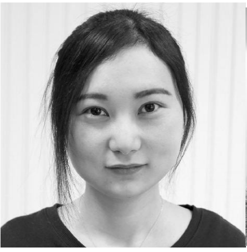


Xiaoyang Guo



Yalan Wang

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Research Areas

❖ Conversion of Natural Gas

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

❖ Industrial catalysis

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

❖ Upgrading of Oil Fractions

- Hydrotreating
- Catalytic reforming/isomerization

❖ Biofuels

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

❖ High Temperature Chemistry

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

❖ Environmental Catalysis

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

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

- **Microstructured Reactors and Membrane Reactors**

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

- **Gas cleaning**
  - Sorbents and processes for H_2S removal.
  - Sorbents and processes for CO_2 capture.

- **Photocatalysis**
  - Water splitting
  - Photo reforming
  - Nitrogen fixation

Main Laboratory Equipment

❖ Reaction Laboratories

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

❖ Catalyst Preparation Laboratory

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

❖ Catalysts and Products Characterization

- Surface area (BET), porosity and pore size distribution
- Chemisorption and adsorption calorimetry
- Temperature programmed methods such as TPR, TPO and TPD, acidity determination by TPD (Altamira BenchCat Hybrid)
- TGA-MS and DSC
- Raman (*ex-situ* and *in-situ*)

- FT-IR (*in-situ*)
- Pyrolysis GC-MS
- GC-MS, micro-GC, MS and HPLC
- XRF – X-ray fluorescence
- Scanning tunneling microscopy (STM)
- The following methods are available at NTNU:
  EM (electron microscopy), XPS (X-ray photoelectron spectroscopy), AES (auger electron spectroscopy), NMR, AFM (atomic force microscopy), ICP-MS and XRD (X-ray diffraction).
- Synchrotron radiation EXAFS and XRD are frequently used through ESRF and other facilities.
- Synchrotron radiation HR-PES and APPES are frequently used through MAXIV, ASTRID2 and other facilities.

Highlights from Activities in 2020

- The Corona pandemic has had a great impact on the activity in 2020, on teaching as well on laboratory work. Group meetings, seminars, etc. have all been digital. As a consequence of travel restrictions, very few has attended international meetings.

- One candidate completed his PhD degree in 2020: Xiaoyang Guo. The title of the dissertation, the title of the trial lecture and pictures of the candidate/committees/supervisors are enclosed.

- 15 M.Sc. students completed their thesis in 2020. Their names and titles of the thesis are enclosed. 2 exchange students also completed their thesis.

- Hilde J. Venvik is appointed as Lise Meitner Guest Professor, Dept. of Chemical Engineering, Lund University, Sweden.

- 56 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).

- Patent applications from group members: Hilde J. Venvik et al. and Jia Yang 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 the academic partners are NTNU, UiO and SINTEF. 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

- iCSI carried out two seminars: a student seminar at Topsøe and the annual seminar at Oscarsborg (Programme is enclosed)

- The group is a research partner in BIO4FUELS, a Centre for Environment - friendly Energy Research (FME), hosted by The Norwegian University of Life Sciences (NMBU). The Center has a total budget of around 270 MNOK over 8 years and covers all important value-chains for conversion of lignocellulosic biomass to biofuels. User partners are key national and international industries, as well as forestry owners and regional authorities. Our activities are related to catalytic processes for production of biofuels and chemicals from biomass.

- The group is involved in several RCN supported research projects with international collaboration such as EMX2025, GAFT, MBCL, H_2MemX, NanoCat4Fuels and KPN Biomass to aviation fuels (B2A). In addition, a project from UK Catalysis HUB has been granted.
- 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: (EHLCATHOL).
- The catalysis group runs a bi-weekly seminar. The programs are enclosed.
- Strategic support from NTNU consisting of PhD scholarships and financial support.

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

Looking back to the 2019 Annual Report, the heading was “Time to refresh”. Well, 2020 did certainly not turn out to be a refreshing year.

The University of Oslo faced more challenges and delays than NTNU, due to longer closures of the labs and generally more restrictions imposed in our capital area. Despite these limitations, iCSI research as such has suffered only moderately from the pandemic due to fortunate timing. Many of our PhD candidates were near completion in 2020, focusing on writing up their research results. Then some new candidates were recruited, and these have manoeuvred impressively well during their start-up phase with course work and supervision via screen.

Educating master’s students is important to the Centre. In 2020, 17 graduating master’s students were associated with iCSI, of which two delivered directly into the ongoing projects. The gender balance within iCSI has been maintained in all personnel categories – within a 40/60 distribution.

In March of last year, just before the lockdown, iCSI welcomed Sebastian Prodinger, a new Postdoctoral fellow, to the University of Oslo. In September three new PhD candidates were welcomed to NTNU: Youri van Valen, Jithin Gopakumar and Wei Zhang. They come from different parts of the world, and you can get to know them better through the interview in the iCSI Annual report.

The high publishing activity has continued from last year, and twelve reviewed papers were accepted and published in 2020. At the end of the year, even more articles were submitted for review. Especially Innovation Area 4 (PVC Value Chain: World Class Energy and Raw Material Efficiency for the Production of Chlorine and Vinyl Chloride Monomer) should be mentioned for the large quantity, but also for the high quality of published articles this year.

The lack of traveling and conference participation is reflected in the list of conference contributions. We were fortunate to be able to hold the iCSI Annual Seminar in September, and 98% of the presentations and posters are from that event. For most of us, this was the only occasion to present research results and for in-person meetings with iCSI partners at other locations.

One exception was the Young Researchers Seminar at the end of February, which was lucky timing. Pablo Beato and Haldor Topsøe hosted the event at their locations in Lyngby. The young researchers were also invited to a tour at the Topsøe catalyst plant in Fredrikssund.

iCSI is proud to have dedicated and enthusiastic international scientific advisors. When they were not able to join our seminar due to travel restrictions, they compensated by holding virtual guest lectures as well as one-to one meetings with four of iCSI's PhD candidates and postdocs. The lectures were highly valued by the industry partners as well.

The representation on the iCSI Board has changed for one of the industry partners in 2020, as Thomas By took over from Johan Skjelstad as K.A. Rasmussen's board representative in August. As of January 2021, Kamilla Jordal replaced Marco Piccinini as Inovyn's representative. iCSI thanks everyone for their efforts during their period on the Board.

Ph.D. Candidates and Postdoctoral Projects

Gold-Bismutite Hybrid Catalysts for Photosynthesis of Ammonia

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

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

The conversion of N_2 to NH_3 in nature at ambient conditions by the nitrogenase enzyme motivates the search for similar sustainable technologies for industrial scale NH_3 production. Photocatalytic ammonia production is one such field gaining popularity owing to the mild reaction conditions at which it allows the reduction of N_2 to NH_3. Bismutite ($Bi_2O_2CO_3$) nanoparticles (NPs) have recently emerged as an important candidate in photocatalysis owing to the alternative $(Bi_2O_2)^{2+}$ and CO_3.

2- layered anisotropic crystal structure, which leads to an internal static electric field thereby facilitating photoinduced charge separation and transfer [1]. However, these NPs have a relatively wide bandgap (~ 3.15 eV) which limits its performance in the visible region of the solar spectrum. Furthermore, the high stability of the N_2 molecule with a bond strength of 941 $kJmol^{-1}$, makes the activation step of N_2 quite challenging at these conditions [3]. Hence, the development of highly efficient photocatalytic materials with improved light harnessing properties have garnered significant research interest.

Gold nanoparticles (Au NPs), owing to their excellent optical properties and localized surface plasmon resonance (LSPR) effect, have emerged as attractive candidates for catalysis and other applications. As a result of the LSPR effect, enhanced field strength of the electromagnetic fields near the surface of Au NPs can be over 500 times larger than the applied field for structures with sharp edges [4]. This may cause heating of the NPs by just absorbing sunlight, which could in turn activate the molecules bonded to the surface. Hence plasmon enhanced photocatalysis would improve the solar energy collection efficiency of semiconductors and is expected to give better yields of ammonia. Recent work by Xiao et al. reported chemical bath deposition of Au NPs on bismutite and studied the same for photocatalytic ammonia synthesis [1]. However, controlling the morphologies of Au NPs is an area that has not yet been explored, and is expected to have a significant effect on the photocatalytic performance.

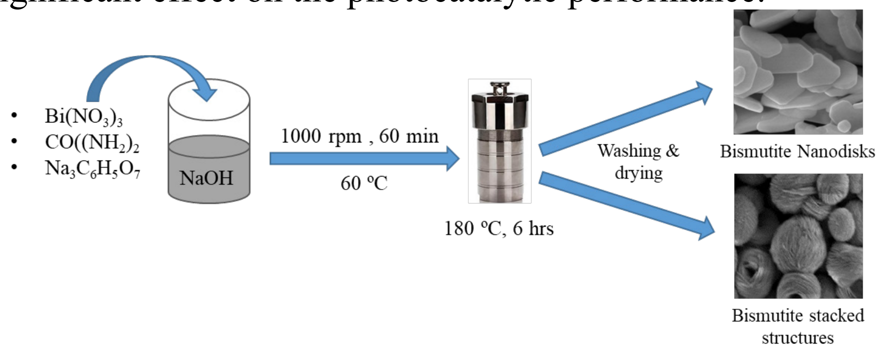

Figure 1 Hydrothermal synthesis route for bismutite NPs

This project aims at synthesizing hybrid NPs of Au with bismutite and to study their performance in photocatalytic nitrogen fixation. Various shapes of bismutite NPs such as disks and 3D stacked structures were synthesized using a facile hydrothermal method as depicted in Figure 1. Au NPs of various shapes will be synthesized using seed-mediated growth in the presence of cetrimonium bromide (CTAB) as surfactant. These particles would then be deposited on the bismutite NPs via different approaches such as photodeposition, ultrasonication among others. The photocatalytic performance of the hybrid catalysts will be studied under simulated solar light. A 300W Xenon arc lamp equipped with AM1.5 filter will be used to irradiate the reactor under N2 purging with 1 sun radiation. Careful optimization of the synthesis route for these Au-bismutite hybrids is anticipated to pave way for a greener and energy efficient photosynthesis of ammonia.

References

[1] C. Xiao, H. Hu, X. Zhang and D. R. MacFarlane, ACS Sustainable Chemistry & Engineering, 2017, 5, 10858-10863

[2] S. Zhang, Y. Zhao, R. Shi, G. I. Waterhouse and T. Zhang, EnergyChem, 2019, 100013.

[3] D. Kumar, S. Pal and S. Krishnamurty, Physical Chemistry Chemical Physics, 2016, 18, 27721-27727.

[4] X. Chen, H. Y. Zhu, J. C. Zhao, Z. F. Zheng and X. P. Gao, Angewandte Chemie International Edition, 2008, 47, 5353-5356.

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

Carbon Nanomaterial-IL Hybrids for Ultrahigh Energy Supercapacitors

Postdoc: Suresh Kannan Balasingam
Supervisor: Prof. De Chen

The project aims to fabricate high energy density supercapacitors using high surface area carbon materials and various ionic liquid electrolytes. In general, supercapacitors having a high power density and low energy density. To increase the energy density of supercapacitors, various strategies have been investigated. Recently, multivalent metal ions-based hybrid capacitors have attracted increased interest since the multivalent ions can more effectively contribute to the redox reactions, which will improve the charge storage capacity and in turn energy density. Due to the earth-abundant nature of zinc metal, zinc-ion based hybrid capacitors have been fabricated using high surface area activated carbon as positive electrodes, pure zinc foil as negative electrodes, and ionic liquids as the electrolyte. Usage of zinc metal foil negatively influences the gravimetric capacitance value, and also there is not enough room for the ionic liquid cations to adsorb on the zinc foil. Therefore, a novel design of carbon-zinc powder mixture has been investigated to replace the heavy zinc foil. The various carbon to zinc mixture ratios, organic and ionic liquid-based electrolytes have been used to fabricate high energy supercapacitors.

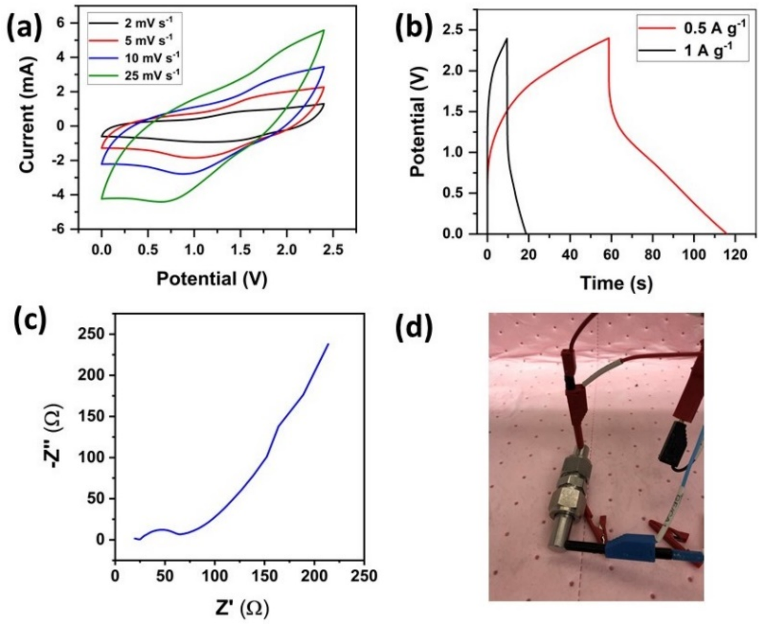

Fig. 1 (a) Cyclic voltammetry curves at different scan rates, (b) Galvanostatic charge-discharge curves at two different current densities, (c) Nyquist plot of electrochemical impedance spectroscopy, and (d) Photograph of Swagelok type-cell

Funding Agency: The Research Council of Norway

Catalysts for NO_x-reduction in maritime transportation

Ph.D. Candidate: Ole Håvik Bjørkedal
Supervisor: Prof. Magnus Rønning

Co-supervisor: Dr. 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 NOx, which must be reduced downstream of the engine. The goal of the project is to develop catalysts for Selective Catalytic Reduction (SCR) under relevant conditions for LNG-propelled ships, as well as reaching a better understanding of the role of the support in SCR-catalysis.

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

The alumina-supported samples were found to have some interesting material properties such as high dispersion for high loading, but the SCR-activity was fairly low, particularly when feeding steam to the reactor. It was suspected that H_2O 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 H_2O was not as drastic for the zirconia-based catalysts. Bimetallic Cu-Fe/ZrO_2 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.

Conference presentations in 2020:

1. Bjørkedal, Ole Håvik; Regli, Samuel K.; Rønning, Magnus. One-Pot Synthesis of Highly Dispersed Mesoporous Fe and Cu Catalysts for NH3-SCR. International Conference on Environmental Catalysis; Manchester (Virtual conference); 2020-09-07 - 2020-09-09 NTNU

Financial support:

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

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 N_2 adsorption, N_2O chemisorption, XRD, TPR, TPD and Raman spectroscopy. Furthermore, the catalysts were tested in the reaction of hydrogenation of hydroxyacetone (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.

Oral presentations:
Cazzolaro Martina, Yang Jia, Beier Matthias Josef, Taarning Esben, Chen De. Catalytic hydrogenation of biomass-derived oxygenates to biochemicals.
- Bio4Fuels Days, December 2020. Virtual meeting.
- NTNU IKP Days, December 2020. Virtual meeting.

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

Catalytic Oxidation of NO to NO_2 For Nitric Acid Production

PhD. Candidate: Jithin Gopakumar
Supervisor: Prof. Magnus Rønning
Co-Supervisor: Dr. Bjørn Christian Enger (SINTEF), Dr. David Waller (Yara) & Dr. Sang Baek Shin (Yara)

Nitric acid is one of the most important industrial chemicals, whose first production dates to the 8th century. Earlier production of nitric acid used potassium nitrates and sulphuric acid as raw materials, which was then replaced by sodium nitrate in 19th century. The present-day commercial production of nitric acid uses a hundred-year-old process called Ostwald process. Wilhelm Ostwald patented these three steps or two stage process in 1902. Several decades of research exists on this process and it has been the cornerstone of many chemical industries to produce the raw material for fertilisers and other chemical commodities.

The Ostwald process comprises of three important chemical steps: (i) Oxidation of Ammonia using Pt/Rh gauzes at high temperature to produce nitric oxide, (ii) A homogeneous gas phase oxidation of nitric oxide to nitrogen dioxide, (iii) Absorption of nitrogen dioxide with water to produce nitric acid.

Conversion of NO to NO_2 is one of the few known third order gas phase reaction, with inverse Arrhenius behaviour. Commercially a series of heat exchangers are used to recover heat and produce NO_2 more economically. Converting this homogeneous gas phase reaction to a catalytic reaction is challenging but beneficial as it leads to (i) significant increase in heat recovery (ii) accelerated oxidation reaction and (iii) substantial decrease in capital expenditure (CAPEX) for new plants.

The thermodynamics of the reaction is favoured by low temperatures whereas catalytic activity is usually favoured by higher temperatures. Additionally, the high concentration of nitric oxide and presence of water in the feed are the main challenges preventing this reaction from being performed catalytically. Hence, to this date there is no catalyst that can convert NO to an extent where equilibrium is attained at industrial conditions.

The first phase of this project concluded with the manganese on zirconia catalyst to be the most promising and, had the catalyst onset temperature to be same for both NO conversion and catalyst reduction. Literature suggests the Manganese (Mn) based catalysts shows good catalytic oxidation for nitric oxide at low temperatures.

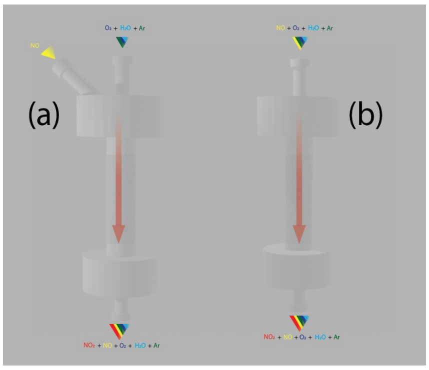

Figure 2(A) MODIFIED REACTOR – NITRIC OXIDE DOSED DIFFERENTLY; AND ((B) OLD REACTOR – NITRIC OXIDE MIXED WITH OTHER REACTANTS

The preferred catalyst working conditions are 200-250◦C and 4 bar pressure. The current work aims to find an efficient catalyst for oxidizing NO to NO2 at these operating conditions Thus, enabling significant process intensification of the nitric acid production plant. A dedicated experimental setup was already built in the first phase of this project, capable of catalytic activity investigation at atmospheric conditions. The major challenge of this project is to reduce the gas phase conversion as much as possible. Hence, the reactor had to be modified initially to dose the NO near the mouth of the reactor to mix the gases closer to the catalyst bed than before (Figure 1)

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An additional goal of this project is to investigate and understand the reaction kinetics and the mechanism of oxidation of NO over promising catalysts. Manganese on zirconia is a promising catalyst and promoting it with noble metals will improve its performance. Platinum shows good catalytic activity without presence of water and silver being popular for formaldehyde production via oxidative dehydrogenation of methanol were two promising candidates as promoters. Another benefit of silver is the ability to decompose N2O upstream of NO oxidation in a nitric acid plant.

A total of six zirconia supported catalysts were made, each with two different loadings of manganese and two promoters (Pt and Ag). The seventh catalyst is 5wt% silver on zirconia, to see the performance of silver alone in comparison to manganese.

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

Material degradation by metal dusting corrosion in compact reformer concepts

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

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

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

The initial stages of carbon formation and metal dusting corrosion of Fe-based Incoloy 800 alloy were studied by SEM and FIB/TEM coupled with EDX/EELS and Raman spectroscopy. The results show that regions on the Incoloy 800 samples subjected to combined near surface severe plastic deformation (NS-SPD) and subsequent thermochemical treatment exhibit no carbon formation, compared with the region not treated by NS-SPD on the same samples. The good corrosion resistance performance is a result of the NS-SPD process producing an ultrafine-grained structure with a higher fraction of grain boundaries together with crystal twinning near the surface. These microstructures increase the effective diffusion coefficient for Cr in the alloy by introducing a higher density of rapid diffusion paths, hence promoting the formation of a thin, protective Cr-rich oxide scale during the thermal treatment, which prevents contact between the carburizing atmosphere and the Fe and Ni contained in the alloy. The results imply that the metal dusting resistance performance of Incoloy 800 in industrial applications can be significantly improved.

Our team is selected for European Institute of Innovation & Technology (EIT) Raw Materials Accelerator Program and Start-up and SME Booster program. Funding of 55,000 Euro was granted to develop innovative products and services that can produce an impact in the raw materials sector and improve the market entry success rate of our team.

Financial support:

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

Three grants awarded from EIT Raw Materials (European Institute of Innovation and Technology, a body of the European Union) for commercialization of the findings from the project.

Publications in 2020:

Xiaoyang Guo. *Inhibiting carbon growth at the initial stage of metal dusting corrosion of high temperature alloys* NTNU PhD thesis, defended 23. June, 2020

Method for reducing metal-dusting corrosion The European Patent Office PCT Patent Application No. PCT/EP2020/075555

Xiaoyang Guo; Estelle Vanhaecke; Jianyu Ma; P.V.D.S. Gunawardana; John C. Walmsley; De Chen and Hilde J. Venvik. *Effects of metal dusting relevant exposures of alloy 601 surfaces on carbon formation and oxide development.* Catalysis Today (2020), in print, https://doi.org/10.1016/j.cattod.2020.04.029.

Xiaoyang Guo; Estelle Vanhaecke; Per Erik Vullum; John C. Walmsley; De Chen and Hilde J. Venvik. *Inhibition of Metal Dusting corrosion on Fe-based alloy by combined near surface severe plastic deformation and thermomechanical treatment,* submitted.

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.

Within these alternatives, the interest in the Fischer-Tropsch Synthesis (FTS) increased in recent years. The FTS converts synthesis gas to hydrocarbons. The selectivity of the FTS can be optimized in order to obtain different products. Among these products, light olefins represent added value compared to fuels, which always will be the main product.

The syngas can be produced from different sources such as natural gas, coal or biomass. One interesting feedstock for the syngas is the biomass. This renewable energy source is abundant and 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. As an example, 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 loses and improve the efficiency of the industries.

In this context, cobalt-based catalysts are going to be studied in the FTS with emphasis on olefin selectivity from syngas derived from biomass, BTL. The catalysts are going to be prepared by different synthesis methods, characterized by several standard and advance techniques, and tested in the FTS. The reaction condition chosen for the project will favor the light olefin production and high conversion.

Due to the selection of fish waste as the initial example as feedstock for the syngas, the initial work plan of this project will be focused on the effect of several components specific to fish waste present in syngas from this source, which could affect the catalytic activity and selectivity. To address these possible catalyst poisons and to improve the catalytic activity and selectivity, different metal oxides and noble metals will be studied as catalysts promoters, as well as different supports. Once the effects of the possible contaminants are analyzed, the catalysts will be tested with real syngas derived from biomass. The last step in the project will be to test the set up with syngas directly from a real gasifier.

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

Catalytic Steam Reforming of Hydrocarbon Impurities from Biomass Gasification

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

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

The PhD project is addressing catalytic steam reforming, converting tars and lighter hydrocarbons to syngas as well as $H_2/CO/CO_2$ ratio adjustment by the water-gas shift reaction as part of this key gas cleaning step. The performance of a series of mixed oxide Ni-Co/Mg(Al)O catalysts prepared from hydrotalcite precursors are currently being investigated.

Presentations in 2020:
Ask Lysne, Kumar R. Rout, Edd A. Blekkan; Catalytic Steam Reforming of Hydrocarbon Impurities from Biomass Gasification. Bio4Fuls Days 2020: Working towards a climate-neutral 2050, November 18-19, 2020, virtual meeting. Oral Presentation.

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

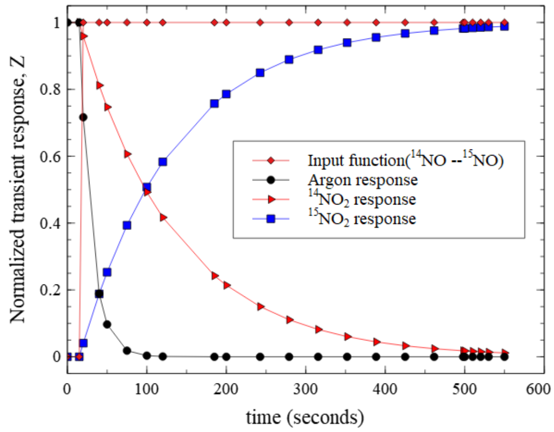
Insights into the kinetics and mechanism of selected industrial catalyzed reactions

Ph.D. Candidate: Moses Mawanga
Supervisor: Prof. Edd Anders Blekkan
Co-supervisor: Assoc. Prof. 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 gas phase at high NO concentration thus requiring long residence times and efficient heat removal. Knowledge of the kinetics and rate mechanism that accurately describe 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 with the objective of having a more intensified process with an added benefit of energy recovery.
The experimental study entails the use of Steady State Intrinsic Transient Kinetic analysis method coupled with a Diffuse Reflectance Infra-red Fourier Transform Spectrometry (SSITKA-DRIFTS) study on a sample of 1 wt% Pt/Al_2O_3 catalyst prepared by incipient wetness impregnation. Reactant gas constitute primary 10 mol% NO and 6 mol% O_2 in Argon to emulate typical industrial conditions within 150–450 °C range and atmospheric pressure conditions at a GHSV of 240,000

ml/g$_{cat}$/h. Upon establishing a steady state reaction rate, the reactant gas was switched from $^{14}NO + O_2$ to $^{15}NO + O_2$ to study the N-containing pathway as well as $NO + {}^{16}O_2$ to $NO + {}^{18}O_2$ to study the O-containing pathway in the formation rates of $^{14}N^{16}O_2$, $^{15}N^{16}O_2$ as well $N^{16}O^{18}O$, $N^{18}O_2$ products respectively.

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



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

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

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

Step 4: $2O* \rightleftharpoons O_2^v + 2*$

Step 5: $2NO + O_2^v \rightleftharpoons NO_2 + *$

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

In another part of the project involves using the adsorption microcalorimetry to measure the heats of adsorption for catalytic activation and functionalization of light alkanes, e.g. using zeolites or metal-exchanged zeolites. Heats of adsorption are indicative of the adsorption energetics and bonding strength of surface species to probe the nature of active sites of the catalyst. With these fundamental experimental data, it will be possible to have a better understanding of the catalytic reactions and thereby use the data for better catalyst design.

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.

Direct synthesis of vinyl chloride from ethylene oxychlorination

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

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 Cl_2 by first chlorinating ethylene to produce EDC, the EDC is then thermally converted to VCM by dehydrochlorination. The HCl produced in the dehydrochlorination reactor is typically captured and recycled to an oxychlorination reactor to convert C_2H_4, O_2, and HCl to EDC, which is again converted to VCM by dehydrochlorination. The balanced VCM process is a complex multi-process including three reaction sections, separation and recycle unites.

The ethylene oxychlorination is typically catalyzed by a promoted $CuCl_2/Al_2O_3$-based catalyst at relatively low temperatures (ca. 220−250 °C) and 2−6 bar. It is not feasible to integrate the low-temperature oxychlorination and high-temperature EDC thermal cracking together, which loses the $CuCl_2/Al_2O_3$-based catalyst stability at high temperatures or reduces the activity of EDC dehydrochlorination at low temperatures.

In the present work, we report an energy-efficient process to produce VCM from ethylene oxychlorination at relatively low temperatures on a metal-free carbon catalyst. To the best of our knowledge, for the first time, a metal-free carbon-based catalyst was reported having the catalytic activity for ethylene oxychlorination to directly produce VCM at a relatively low temperature of 250 °C. We found that the N-doped carbon catalyst not only catalyzes the ethylene oxychlorination but also facilitates the EDC dehydrochlorination reaction due to the bifunctional ability. The oxychlorination-dehydrochlorination process was integrated into one dual-bed single pass reactor, where ethylene oxychlorination catalysts were followed by N-doped carbon catalysts, at a low temperature (250 °C) to achieve a high VCM yield up to 76%, even higher than the one in the current industrial single-pass balanced VCM process. The one-pot process has been remarkably intensified by a synergic effect between the oxychlorination and dehydrochlorination reactions at the same type of active site by the surface Cl* looping between the two reactions.

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

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

PhD candidate: Jianyu Ma
Postdoc.: Dr. Mehdi Mahmoodinia
Supervisors: Prof. Edd A. Blekkan, co-supervisor Dr. Kumar R. Rout, SINTEF.

Bioenergy is a significant contributor to the renewable energy supply in Norway, today mainly used for heating. Syngas from biomass gasification can be used for electricity production or chemical synthesis to produce synthetic fuels. However, it is a complex gas mixture including H_2, CO, CO_2, H_2O, CH_4 , H_2S and other sulfur-containing species, which can corrode downstream equipment, and also poison catalysts used for fuel synthesis. Hence, sulfur removal from gas streams is an important step for utilizing biomass for energy production.

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

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

Publications and presentations in 2020:
Mahmoodinia Mehdi; Ma, Jianyu; Sauer, Maximilian; Kumar Ranjan; Blekkan, Edd Anders: Performance of manganese-based solid sorbents for H_2S removal: Particle size and promoter effects on sorbent capacity, iCSI annual seminar; Drøbak, Oslo, 2020-09-14 - 2020-09-15.
Ma, Jianyu; Rout, Kumar Ranjan; Sauer, Maximilian; Mahmoodinia, Mehdi; Blekkan, Edd Anders. Investigations of molybdenum-promoted manganese-based solid sorbents for H2S capture. Biomass & Bioenergy 2020; Volume 143. 105843.
Ma, Jianyu, PhD Thesis: High-temperature desulfurization of biomass-derived synthesis gas using solid sorbents, 26.01.2021.

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 H_2 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 H_2 dissociation. After dissociation, diffusion of hydrogen atoms to sites with higher adsorption strength on the flat terrace is facile, making it available for hydrogenation reactions.

The 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 recontruction 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.

Publications and Conference contributions:

Weststrate, C.J. (Kees-Jan); Mahmoodinia, M.; Farstad, M.H.; Svenum, I.-H.; Strømsheim, M.D.; Niemantsverdriet, J.W. (Hans); Venvik, H.J., Interaction of Hydrogen with Flat (0001) and Corrugated (11–20) and (10–12) Cobalt Surfaces: Insights from Experiment and Theory. Catalysis Today, 342 (2020) 124–130. https://doi.org/10.1016/j.cattod.2019.04.002.

Marie Døvre Strømsheim, Ingeborg-Helene Svenum, Mari Helene Farstad, C. J. Kees-Jan Weststrate, Anne Borg, and Hilde Johnsen Venvik, CO-Induced Surface Reconstruction of the Co(11–20) Surface—A Combined Theoretical and Experimental Investigation, The Journal of Physical Chemistry C 2020 124 (52), 28488-28499. DOI: 10.1021/acs.jpcc.0c07852

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:

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

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

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

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

Development of catalyst for biomass to aviation fuels

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

The aviation sector heavily relies on fossil fuels and thereby, contributing to global warming. This forced human community to search for an alternative fuel which is renewable, abundant and carbon neutral emitter. The biomass is the key resource which satisfies all these qualities. The government, industry and research community have now collaborated to investigate the conversion of biomass to fuel.

At present, 80% of the global energy demand is satisfied by the fossil fuels, in particular 90% of the transport energy consumption. The transport sector requires dramatic emissions slash in the carbon-neutral scenario, from about 80 million tons of CO_2 ($MtCO_2$) in 2013 to just over 10 $MtCO_2$ in 2050. It should be noted that aviation and marine transportation is large CO_2 emission resources, which has a share of global CO_2 emission about 4-5%. The aviation industry is interested in utilizing the bio derived aviation fuel to tackle the challenge. Additional challenge is to satisfies the strict critical requirements of the jet-fuel properties.

The PhD project focus on the theme to produce two cheap catalyst which is active in carbon-carbon coupling and HDO reaction resp. The novelty here lies in the process developed specifically for allowing an economically means to produce bio-jet fuel. The ultimate goal is to produce jet-fuel from biomass in a price range (<0.78 Euro/L) competitive to the present state of art minimum fuel selling price reported in the literature from biomass (1.04 Euro/L) via fast pyrolysis. The key here is to increase the carbon retention with reduced oxygen content in the final bio-oil through ex-situ tandem configuration of carbon-carbon coupling and hydro-deoxygenation catalyst after fast hydropyrolysis of biomass.

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Publication in 2021:
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Financial support: The Research Council of Norway

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 CO_2 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 with synchrotron radiation, X-ray diffraction, UV-Vis spectroscopy, Fourier-transform infrared spectroscopy and Raman spectroscopy. New insight on the active sites of the catalysts and the respective kinetics of the chemical reactions can guide towards favorable compositions and conditions for sustainable process industry.

Financial Support:
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Oral presentations 2020:
Regli SK, Rønning M. Invited talk "Multivariate statistical analysis of in situ and operando X-ray Absorption Spectroscopy data". ESRF User Meeting 2020, Grenoble, France.

Bjørkedal, Ole Håvik; Regli, Samuel K.; Rønning, Magnus. (2020) One-Pot Synthesis of Highly Dispersed Mesoporous Fe and Cu Catalysts for NH_3-SCR. International Conference on Environmental Catalysis. University of Manchester; 2020-09-07 - 2020-09-09.

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

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

It is well-known that the largest amount of CO_2 emissions comes from fossil fuel power plants, and because of its destructive effect on the global climate, urgent actions must be considered. One of it is CO_2 capture and storage (CCS) which is an intensively researched area aimed at mitigating the CO_2 release into atmosphere. Due to the increase of total natural gas/coal generated electrical power ratio, the project scope is focused on designing CO_2 sorbents for post-combustion natural gas combined cycle (NGCC) power plants. In addition, a cost-effective retrofit can be implemented for the existing power plants.
Various technologies and materials have been developed and investigated, especially the aqueous alkanolamines scrubbing of CO_2. However, the large water content used in this process rises the energy consumption amount, and the direct contact of the amine solution with the equipment requires anti-corrosive

materials which are very expensive. Accordingly, amine functionalized solid sorbents are proposed for this project. By anchoring the amine containing material on the pore surface of the support, the amine-equipment contact is avoided. Furthermore, less energy is consumed because no water is involved in the chemisorption process. If comparing with the monoethanolamine NGCC integrated process, a cost saving of 25-30% is estimated by using solid sorbents. Nevertheless, the amine functionalized solid adsorbents have also some drawbacks like reduced capacity at low CO_2 partial pressure and low chemical and thermal stability. Herein, polyethyleneimine (PEI) and penthaethylenehexamine (PEHA) have been used as initial materials for chemisorption. They are described by a very high amine density, an important property required to achieve a high CO_2 adsorption capacity. Moreover, their large molecular weight, especially the one of PEI, increases their resistance to high adsorption-desorption temperatures. However, a very high molecular weight is unwanted because it is difficult to impregnate into the pores. Furthermore, a highly viscous material also involves a very hydrogen bonded environment ($\mathrm{CH_3NH_2: \cdots H - NH - CH_3}$), which minimizes the CO_2 diffusion to the amine sites. The diffusion is also decreased by the high amine loadings. In order to develop large loadings, supports with enough pore volume and pore size are required. In this work, silica supports are used due to their thermal and mechanical stability. The crosslinking and support bonding of amines concepts are also considered in order to avoid amine loss.

To store pure CO_2, the adsorption process should be very selective, and the desorption step should be realized in pure CO_2. As the process is designed based on temperature swing adsorption, a desorption step in pure CO_2 and high temperature deactivate very fast the amines because of the ureas formation. 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. Besides the impressive chemical stability, the final adsorbent is also thermically 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.

Presentations in 2019:

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

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

Design of low-cost and carbon-resistant Ni-based mesoporous silicas for chemical CO_2 utilization through tri-reforming of methane

Postdoc: Katarzyna Świrk
Supervisor: Prof. Magnus Rønning

The carbon capture and utilization (CCU) processes have gained significant attention as a potential strategy to reduce greenhouse gas emissions from major industrial emitters. Tri-reforming of methane (TRM) is viewed as a part of these technologies, which allows simultaneous conversion of CO_2, CH_4, H_2O, and O_2 into synthesis gas (H_2/CO ca. 1.5 - 2.0). The process is a combination of three main reforming reactions that take place in a single reactor; steam reforming of methane (SRM), dry reforming of methane (DRM), and partial oxidation of methane (POM) [1,2]. Accordingly, carbon dioxide is treated as a source of carbon for chemicals and fuels feedstock. TRM has not yet been established on an industrial scale. It is a complex process, requiring an active and stable catalyst that would be resistant to deactivation caused by sintering, active site oxidation, or carbon formation [3]. Therefore, a lack of efficient catalysts has prevented the tri-reforming of methane from making a bigger impact.

The EU-funded Marie Skłodowska-Curie Individual Fellowship, MesoSi-CO_2 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 (N_2 sorption, H_2 chemisorption, XRD, XRF, TGA/DSC-MS, DRIFT). 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 University in Paris, France.

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catalytic production of industrially useful synthesis gas with desired H_2/CO ratios. Catalysis Today, 2004;98:463. doi:10.1016/j.cattod.2004.09.054.
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Publications:

1. Katarzyna Świrk, Hailong Zhang, Shanshan Li, Yaoqiang Chen, Magnus Rønning, Monika Motak, Teresa Grzybek, Patrick Da Costa, Carbon-resistant NiO-Y_2O_3-nanostructured catalysts derived from double-layered hydroxides for dry reforming of methane, Catalysis Today, 2020; Article in press. doi:10.1016/j.cattod.2020.03.032
2. 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 CO_2 to methane, International Journal of Hydrogen Energy, 2020; Article in press. doi:10.1016/j.ijhydene.2020.03.202
3. Katarzyna Świrk, Magnus Rønning, Monika Motak, Teresa Grzybek, Patrick Da Costa, Synthesis strategies of Zr- and Y-promoted mixed oxides derived from double-layered hydroxides for syngas production via dry reforming of methane, International Journal of Hydrogen Energy, 2020; Article in press. doi:10.1016/j.ijhydene.2020.04.239
4. Katarzyna Świrk, Jacek Grams, Monika Motak, Patrick Da Costa, Teresa Grzybek, Understanding of tri-reforming of methane over Ni/Mg/Al hydrotalcite-derived catalyst for CO_2 utilization from flue gases from natural gas-fired power plants, Journal of CO2 Utilization, 2020;42:101317. doi: 10.1016/ j.jcou.2020.101317

Oral presentations:

1. Katarzyna Świrk, Abdelali Zaki, Karim Adil, Gérard Delahay, Amandine Cadiau
Facile modifications of HKUST-1 by Mn, Nb and V for low-temperature selective catalytic reduction of nitrogen oxides by NH_3, 11th International Conference on Environmental Catalysis – ICEC 2020, 6th - 9th September 2020, Manchester, UK (due to coronavirus situation the conference was held virtually).
2. Katarzyna Świrk, Hailong Zhang, Shanshan Li, Yaoqiang Chen, Magnus Rønning, Monika Motak, Teresa Grzybek, Patrick Da Costa,
Carbon-resistant NiO-Y_2O_3-nanostructured catalysts derived from double-layered hydroxides for syngas production via dry reforming of methane, 11th

International Conference on Environmental Catalysis – ICEC 2020, 6th - 9th September 2020, Manchester, UK (due to coronavirus situation the conference was held virtually).

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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:
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Advanced characterization of Pd-based membrane model systems

Postdoc: Marie D. Strømsheim
Project organization: Professor Hilde J. Venvik, Adj. Associate Professor Ingeborg-Helene Svenum (SINTEF), Dr. Thijs Peters (SINTEF), Dr. Marie Døvre Strømsheim (postdoc)

The postdoctoral work is part of H_2MemX, 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). The focus of the postdoctoral project is 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. The overall aim is to apply the knowledge of segregation phenomena and changes in surface chemistry and composition under these conditions 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 (Pd75Ag25(100) and Pd75Ag25(111) 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 mbar total pressure.
Repeated cycles of CO oxidation (ramping the temperature up and down between 30 °C and 450 or 600 °C in 10:1 O_2:CO and ~1 mbar total pressure), over a Pd75Ag25(100) single crystal was performed whilst monitoring the Pd 3d and Ag 3d core levels. The results showed that the relative amount of Pd decreased upon heating as the CO coverage was lifted. However, the segregation demonstrated a degree of reversibility. Furthermore, a higher amount of Pd in the surface was found at 30 °C prior to ramping the temperature, in comparison to the amount of surface Pd upon returning to 30 °C. The higher amount of surface Pd before the temperature cycles was attributed to the time spent with high CO coverage between the cycles. Similar investigations of segregation under repeated CO oxidation cycles (10:1 O_2:CO) were recently performed over Pd75Ag25(111) and Pd(111) single crystals.

Acknowledment:
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. 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 and Conference contributions:
Marie D. Strømsheim, Ingeborg-Helene Svenum, Mehdi Mahmoodinia, Virginia Boix, Jan Knudsen, Hilde J. Venvik, Investigations of the surface dynamics of Pd-alloy surfaces under oxidation reactions, oral contribution at the 11th International Conference on Environmental Catalysis (ICEC2020), 9th of September 2020.
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, accepted.

Alginate as a precursor for highly dispersed carbon-supported catalysts

Ph.D. Candidate:	Joakim Tafjord
Supervisor:	Assoc. Prof. Jia Yang
Co-supervisors:	Prof. Em. Anders Holmen, Prof. Em. Erling Rytter and Research Scientist Rune Myrstad

Global warming and depletion of oil reserves has strengthened the interest of development of processes that can replace the use of crude oil. One alternative is the catalytic process known as Fischer-Tropsch synthesis (FTS). In this reaction, syngas ($CO+H_2$) reacts to form a range of hydrocarbons, such as light olefins, gasoline, diesel, and waxes, and water as a by-product. Among these hydrocarbons, the lower olefins (C2-C4) and their derivatives are important building blocks in the chemical industry.

The renewability of FTS can be increased by utilizing syngas that originates from biomass. However, biomass-derived syngas is lean in hydrogen, and must be supplied with additional hydrogen for employment in FTS. For this reason, iron is an attractive metal for FTS catalysts, as they are catalytically active for both FTS and the water-gas shift (WGS) reaction. Through the latter, hydrogen can be produced by a reaction between CO and H_2O.

Alginate is an abundant biopolymer found in brown algae. This project aims to employ alginate 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 synthesis parameters are tuned to achieve material characteristics that are advantageous for highly active catalysts. The investigated metals are Fe, Co, Ni, and Cu, but the focus is on Fe-catalysts and the tuning of material properties to optimize 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 of the pyrolysis process (FTIR, XAS, XRD), and during FTS (XAS, XRD, Mössbauer) to study how different activation procedures and the addition of promoters affect the catalyst characteristics and performance.

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

Process design and optimization of biorefineries for catalytic upgrading of pyrolysis-based bio- oils.

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 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 H_2O, instead of CO_2, which is common now. 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

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

PhD. Candidate: Mario Ernesto Casalegno
Researcher: Dr. Nikolaos Tsakoumis
Supervisors: Prof. De Chen and Prof. Edd A. Blekkan

The transition towards more sustainable means of energy production, distribution and use is a key issue. Slowing down, or even reversing the negative climatic effects from the utilization of fossil fuels is the ultimate goal. Utilization of H_2 as an energy carrier can be a sustainable solution that will reduce the impact of human activities on the environment. Provided that H_2 is produced in a sustainable way from renewable sources, such as water (using renewable energy) or biomass, it has the potential through its use in fuel cells with favorable efficiencies to cover energy needs with a significant reduction in greenhouse gas emissions. Steam reforming of hydrocarbons is a mature technology for H_2 production. Bioethanol formed by fermentation processes has significant advantages and appears to be a strong candidate as an energy vector suitable for H_2 production.

Our efforts in this project are focusing on the creation of a prototype that integrates steam reforming of bioethanol for H_2 production with CO_2 separation and H_2 combustion into a compact multichannel reactor that can be used on-board vehicles 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.

Other activity in 2020:
N.E. Tsakoumis, A. Baklezos, I. Vardiambasis, T. Kapetanakis, C. Nikolopoulos. (2020) Fluxgate Configuration for Obtaining Magnetic Properties of Catalytic Nanoparticles: A Feasibility Study. 2020 IEEE International Instrumentation and Measurement Technology Conference (I2MTC). IEEE Instrumentation and Measurement Society; Dubrovnik, Croatia, 25-28 May 2020.

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 Knowledge-based development for Energy applications) is an MSCA-ITN project involving 17 European partners. The main objective is to train young scientists to master and combine various state-of-the-art methodologies for the rational development of bimetallic catalysts to improve the current renewable raw materials conversion to hydrogen and implement them in an industrial context.

The BIKE approach will be applied to three industrially relevant hydrogen production processes: Steam reforming of biogas/biomethane, aqueous phase reforming of liquid renewable feedstock, and anion exchange membrane water electrolysis. Addressing to evaluate, exploit and validate the next generation of the bimetallic catalysts under various conditions such as high, low temperatures, in the presence of steam, water, alkaline media, among others.

At NTNU, we will focus our research on aqueous phase reforming (APR), described as an alternative to the traditional steam reforming. APR can be used to convert streams of low value mixed polyols to H_2 and CO_2. It is carried out at low temperatures (200-300°C) in the presence of liquid pressurized water, conditions that favour hydrogen formation and decrease undesirable decomposition reactions.

The high functionality of the biomass used as a feedstock on the APR process leads to the formation of non-desired products that reduce the overall yield and affect the catalyst stability [1]. In APR conditions, selectivity challenges on the catalyst surface decrease the hydrogen production: consecutive reactions occur, such as methanation and Fisher-Tropsch synthesis, producing methane and alkanes [2]. The selectivity can be tuned to produce H_2 as a function of the active metal, the catalyst support, the nature of the feed, and process conditions.

An interesting approach to improve the properties of the catalyst is by adding a second metal to form bimetallic systems. In APR, the synergistic effects of bi-metallics catalyst can enhance the performance, such as increasing H_2 selectivity or improving the catalyst's thermal stability by enhancing the dispersion and interaction of the metals with the support [3]. For example, the addition of Ni or Co to a platinum-based catalyst significantly increases the turnover frequency of H_2 production, maintaining a high H_2 selectivity compared to the platinum-based catalyst [4]

In this project, we will 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. We will study bimetallic 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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Partial oxidation of methanol to formaldehyde over silver

PhD Candidates: Stine Lervold, Youri van Valen (New PhD, started August 2020)
Supervisor: Prof. Hilde J. Venvik
Co-supervisors: Senior Scientist Dr.ing Rune Lødeng (SINTEF), Assoc. Professor Jia Yang.

Formaldehyde is a reactive C_1 chemical building block with numerous applications, most notably in the production of wood adhesives and fine chemicals. Formaldehyde is made through the selective partial oxidation of methanol. Industrially formaldehyde is produced via several processes, mainly utilizing either a silver catalyst or a catalyst based on mixture of iron and molybdenum or vanadium oxides. Dynea AS owns both processes and recognizes the economic potential of the silver catalysed process. The main objective is to increase the overall yield of the process and increase the lifetime of the silver catalyst.

The PhD projects aim to create a better understanding of what happens to the surface and chemical composition of the Ag catalyst over the course of its lifetime and how this is linked to the activity and stability of the catalyst. An experimental protocol has been developed based on the concept of an annular reactor. The annular reactor design offers a controlled system in with isothermal conditions, laminar flow, and suppresses gas phase interactions. Next to this there are seemingly negligible mass transfer limitations. This protocol has allowed for running the methanol to formaldehyde (MTF) process at low conversion with excess oxygen. As such kinetic data of surface reactions can be extracted at near industrial conditions. These activities will continue going forward into the next PhD period. Next to kinetic data there is interest in gathering data on how the catalyst surface develops over time, and how this surface development affects the reaction kinetics. The catalysts will be analysed using various techniques, such as XRD and SEM, with the ability to utilise advanced techniques within iCSI (FIB/TEM) and in collaboration with MAXIV, Lund University (in situ hard X-ray ptychography and limited angle ptychographic computed tomography). Results from the experiments will be shared with the research partners within iCSI to aid in their research activities into this process.

Funding: 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).

DFT investigation on promoter effects in $CuCl_2/\gamma$-Al_2O_3 catalyzed ethylene oxychlorination

Postdoctoral fellow: Yalan Wang
Supervisor: Prof. De Chen

Ethylene oxychlorination is an important process to produce ethylene dichloride, vinyl chloride monomer and polyvinyl chloride. CuCl2/γ-Al2O3 is identified as a superior catalyst for ethylene oxychlorination. However, the CuCl2/γ-Al_2O_3 catalyst is prone to deactivation by sublimation and agglomeration of the copper (I) chloride (CuCl) phase. To reduce this phenomenon, promoters are normally added in the catalyst to maintain and enhance the activity and stability. Although the addition of promoters exhibits better performance, the exact mechanism of the promoter effect remains unclear. In this work, DFT calculations were used to gain insight into the promoter effect, with LiCl, NaCl, KCl, RbCl, CsCl, $BeCl_2$, $MgCl_2$, $CaCl_2$, $SrCl_2$, and $BaCl_2$ as promoters on $3CuCl_2/\gamma$-$Al_2O_3(110)$. Two types of adsorption structures were obtained. Type 1 includes Na-, K-, Rb-, Cs-, Ba-, and Sr-doped $CuCl_2$ catalysts. Type 2 includes Li-, Ca-, Mg-, and Be-doped $CuCl_2$ catalysts. The formation energy of Cl vacancy was analyzed firstly, which can be directly correlated to charge of Cl as well as promoter ionization energy, based on the two types of adsorption structures. The analysis of adsorption

structures illustrates that all promoters can form bond with $CuCl_2$, which changes the electronic properties of $CuCl_2$, therefore the formation energy of Cl vacancy. DFT was then used to calculate the total reaction cycle of ethylene oxychlorination, which includes three steps, namely reduction, oxidation, and hydrochlorination. The group IA elements in type 1, namely Na-, K-, Rb-, and Cs-doped catalysts, were selected to investigate the reduction and oxidation, respectively, since they were considered as the rate determining steps (RDSs). It is found that both the reduction barrier and oxidation barrier were related to formation energy of Cl vacancy, as well as charge of Cl and promoter ionization energy. The reduction barrier follows CsCl > RbCl > KCl > NaCl, while the oxidation barrier follows the reverse tendency CsCl < RbCl < KCl < NaCl. K-doped catalyst displays better performance by taking into account both reduction and oxidation steps.
The three steps reaction cycle on undoped $CuCl_2$ catalyst and K-doped $CuCl_2$ catalyst were investigated subsequently. It was found that both catalysts can go back to the original surface after the reaction cycle. For undoped $CuCl_2$ catalyst, O_2 dissociation is the RDS, with dissociation barrier as 0.82 eV. While for K-doped $CuCl_2$ catalyst, EDC desorption is the RDS, with desorption barrier as 0.44 eV. It can be concluded that addition of K reduces the O_2 dissociation barrier but increases EDC desorption barrier. The RDS is changed from O_2 dissociation to EDC desorption. The conclusion is in good agreement with experiments. The calculation gives the insight of K effect on $CuCl_2/\gamma\text{-}Al_2O_3$ catalyzed ethylene oxychlorination.

Publications in 2020:
[1] Y. Wang, L. Xiao, Y. Qi, J. Yang, Y. Zhu, and D. Chen, J. Phys. Chem. C 2020, 124, 2501–2512.
[2] H. Ma, Y. Wang, Y. Qi, K.R. Rout, and D. Chen, ACS Catal. 2020, 10, 9299–9319.

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

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 H_2 separation on a side stream of the Equinor Methanol plant at Tjeldbergodden, Norway. Ultra-pure H_2 is produced, while at the same time, CO_2 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. CO_2 has little impact by competitive adsorption, but its total effects on the surface reaction chemistry remain to be understood. NH_3, as a potential C-free energy storage and carrier, should also be taken into consideration. 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 har 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).

Mechanism and Kinetics of Byproducts Formation in Ethylene Oxychlorination

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

Oxychlorination of ethylene oxychlorination to 1,2-dichloroethane (EDC) is a crucial step in the production of Polyvinyl chloride (PVC), one of the most commonly used plastic materials. PVC is obtained by the polymerization of vinyl chloride monomer (VCM), which can be produced from ethylene through a two-step process involving ethylene chlorination to EDC, followed by the thermal cracking of EDC to VCM. To date, the ethylene route is predominant, and based on that more than 90% of the VCM production plants worldwide are using the balanced VCM process. Industrial oxychlorination catalysts consist of $CuCl_2$ supported on γ-Al_2O_3 and promoted with various dopants, which are very selective (ca. 93−99%) in the typical temperature range of 473−733 K using fluid or fixed bed reactors.1,2

A deep understanding from the molecular level on the kinetics and the determination of structure-activity relationships has the fundamental meaning in the development of the heterogeneously catalyzed process. In our previous articles, based on the three-step redox in a Mars–van Krevelent (MvK) mechanism, the kinetic modeling of neat $CuCl_2/Al_2O_3$ and K-doped $CuCl_2/Al_2O_3$ for ethylene oxychlorination, but many possible and potential correlations still need to be studied further.3

In ethylene oxychlorination, a series of side reactions can accompany, leading to the production of chlorocarbons and carbon oxides (Figure 10), thus inevitably decreasing EDC selectivity. And the selectivity determines the technology and finally affects the economic efficiency of the process. However, such knowledge is limited in byproducts of ethylene oxychlorination because of the complex reaction network. Therefore, our aim of this project is that, by using some specific techniques, like UV-Vis, XPS, GC-MS, Synchrotron, and so on, building a kinetic model of the sub-network and integrate the sub-network kinetic model to the whole network. Besides, we plan to validate the kinetic model of the whole network by experiments at industrially relevant conditions (high conversion of ethylene and oxygen at NTNU lab, high-pressure HCl experiments at INNOVY lab. Based on experimental results, DFT study, new catalysts will be designed, in terms of catalyst support, co-promoters. And the catalyst will be tested and optimized. This work is concentrating on gaining a better understanding of the reaction and developing more efficient catalysts.

Publications:

[1] Lin, Ronghe, Amol P. Amrute, and Javier Pérez-Ramírez. "Halogen-mediated conversion of hydrocarbons to commodities." Chemical reviews 117.5 (2017): 4182-4247.

[2] Ma, Hongfei, et al. "Critical Review of Catalysis for Ethylene Oxychlorination." ACS Catalysis 10.16 (2020): 9299-9319.
[3] Ma, Hongfei, et al. "Kinetic modeling of dynamic changing active sites in a Mars-van Krevelen type reaction: Ethylene oxychlorination on K-doped $CuCl_2/Al_2O_3$." Chemical Engineering Journal 407 (2021): 128013.

Enhanced visible light absorption TiO_2 based catalysts for photocatalytic H_2 generation

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

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

Titanium dioxide (TiO_2) is n-type ideal semiconductor photocatalysts, which is being widely used in H_2 production, environmental purification, self-cleaning, CO_2 reduction, organic synthesis and solar cells due to high thermal stability, cost-effective, nontoxic and environmentally friendly. Due to the wide band gap (3.2 eV) of TiO_2, it can only absorb UV light up to 380 nm, which is an intrinsic limitation for the TiO_2-based photocatalysts to efficient light harvesting. The charge separation efficiency is a crucial factor for the efficient photocatalytic activity of TiO_2. In spite of its versatility, the mobility of electrons in TiO_2 is low which affects the electron transport rate leading to a decrease in the collection efficiency of the photogenerated electrons. Numerous TiO_2 based photocatalysts have developed for half photocatalytic reaction for H_2 by using the sacrificial reagents by utilizing the photogenerated electrons in the conduction band. These inorganic sacrificial reagents can be easily oxidized to produce different harmful products by the photogenerated holes and promote the H_2 production reaction and making the photocatalytic system expensive. Till the time, there is no such catalysts available with a stat of the art efficiency, selectivity and stability along with the efficient and ideal photoreduction setup.

In this project, to overcome the above-mentioned problem, various approaches like heterojunction formation of TiO_2 with narrow band gap semiconductor in core-shell formate, doping of heteroatom, application of co-catalysts will be applied to increase the photocatalytic activity of semiconductor materials (TiO_2) which are thermally stable, abundance, cost effective and biocompatibility.

Publications:

Muhammad Zubair, Ingeborg-Helene Svenum, Magnus Rønning, and Jia Yang, Facile synthesis approach for core-shell TiO_2–CdS nanoparticles for enhanced photocatalytic H_2 generation from water", Catalysis Today, 328 (2019) 15-20.

Ata ul Rauf Salman, Signe Marit Hyrve, Samuel Konrad Regli, Muhammad Zubair, Bjørn Christian Enger, Rune Lødeng, David Waller and Magnus Rønning, "Catalytic oxidation of NO over $LaCo1\text{-}xB_xO_3$ (B =Mn, Ni) perovskites for nitric acid production", catalysts, 9 (2019), 429

Muhammad Zubair, Ingeborg-Helene Svenum, Magnus Rønning, and Jia Yang, "Core-shell nanostructures of graphene-wrapped CdS nanoparticles and TiO_2 ($CdS@G@TiO_2$): The role of graphene in enhanced photocatalytic H2 generation", Catalysts, 10 (2020), 358.

Muhammad Zubair, Estelle Marie M. Vanhaecke, Ingeborg-Helene Svenum, Magnus Rønning, and Jia Yang, "Core-shell particles of C-doped CdS and graphene: A noble metal-free approach for efficient photocatalytic H_2 generation", Green Energy & Environment, 5 (2020) 461-472

Oral Presentations:

1: Muhammad Zubair, Magnus Rønning, and Jia Yang, "Core-shell nanostructures of graphene wrapped CdS nanoparticles and TiO_2 ($CdS@G@TiO_2$): The role of graphene in achieving enhanced photocatalytic H_2 generation", The Norwegian Catalysis Symposium 2019, 5-6 December 2019, Bergen, Norway

2: Muhammad Zubair, Magnus Rønning, and Jia Yang, "Core-shell nanostructures of graphene wrapped CdS nanoparticles and TiO_2 ($CdS@G@TiO_2$)", 1st meeting of the Norwegian NanoSymposium, 16-17 October 2019, Trondheim, Norway

3: Muhammad Zubair, Magnus Rønning, and Jia Yang, "Core-shell nanostructures of graphene wrapped CdS nanoparticles and TiO_2

($CdS@G@TiO_2$) for enhanced photocatalytic H2 generation", European Material Research Society (E-MRS) spring meeting, 26-31 May 2019, Nice, France
4: Muhammad Zubair, Magnus Rønning, and Jia Yang, "Artificial photosynthesis for H_2 generation from water employing $CdS@TiO_2$ nanostructures", Norwegian Academy of Technological Sciences, 26 March 2019, Trondheim, Norway.

Financial support: The Ph.D. research work is financially supported by NTNU through strategic funding support.

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

Exchange Ph.D. student: Hao Zhang
Supervisor: Prof. De Chen
Co-supervisor: Dr. Navaneethan Muthuswamy

Proton-exchange membrane fuel cells (PEMFC) have showed great prospect in transportation by eliminating the emission of green house gases, but their wide application is limited by the lack of cost-effective cathodic electrocatalysts for ORR. The integration of carbon support and well-designed Pt-based bimetallic nanoparticles is considered as a promising way to solve this problem. In this project, carbon nanofiber (CNF) will be used as support materials due to the combined advantages of electronic conductivity, high surface area and stability. On the other hand, the specific structures of Pt combining with transition metal Co involve intermetallic alloy and core-shell structure, which not only reduces the usage of Pt but also improves the inherent activity of Pt sites under the effect of metal-metal interaction and lattice strain.

Firstly, the single Pt nanoparticles supported on CNF were prepared by an ex-situ colloidal synthesis method. In this method, the size of Pt nanoparticles is controlled in the colloidal solution before depositing on the corresponding supports. Electrochemical measurements were performed in a three-electrode system with a rotating disk glassy carbon electrode connected to a potentiostat. The ORR-activities were determined by performing linear sweep voltammetry (LSV) from 1.1V to 0.01V at a sweep rate of 5mVs-1 in an O_2-saturated 0.1 M HClO4 electrolyte, with a rotating speed of 1600 rpm. The ORR mass activity for Pt/pCNF (25 wt%) shows 0.085 A/mgPt at 0.9 V which is much lower than the target (0.44 A/mgPGM) set by DOE for platinum group metal catalysts, but is higher than commercial 30 wt% Pt/C (0.075 A/mgPGM).

In future work, the bimetallic nanoparticles supported on CNF including PtCo alloy and PtCo core-shell structure will be prepared and tested. Characterization including TEM, XPS, EXAFS and XANES will also be done to understand the catalysts behavior for the above electrochemical reactions.

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

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

Volatile organic compounds (VOCs), emitted from a variety of industrial processes and transportation activities, are considered as an important class of air pollutants. Catalytic oxidation is one of the most developed techniques used for the elimination of VOCs, as it requires lower temperatures than thermal oxidation. Herein, we choose the toluene as VOCs probe molecule because aromatics are present in the industrial and automotive emissions. Typical catalysts for toluene oxidation are mainly noble metals, which have high activity at low temperatures, while they are costly. Metal oxides (Fe, Cr, Cu, Mn and Co) are a cheaper alternative to noble metals as catalysts for VOC oxidation. They present sufficient activity, although they are less active than noble metals

at low temperatures. Cu mixed metal oxides catalysts are effective oxidation catalysts due to their high oxygen storage capacity and facile Cu/Cu^{2+} redox cycle. On the other hand, catalysis is a kinetic phenomenon, the toluene total oxidation reaction is the combination of the reduction and oxidation of the catalysts, and the detail reaction mechanism, as well as its active sites, are not yet fully understand.

In the present work, we comparatively studied the toluene oxidation on the Cu/Al_2O_3 and Cu/TiO_2 catalysts to understand the oxygen vacancy dependent reaction activity. Based on our group's previous research, with the help of the in-situ UV-Vis-NIR spectrometry and MS data, the step transient and steady-state operando kinetic studies can provide the exact information of the transformation of Cu species, quantify the change of oxygen vacancies and the corresponding reaction rate. The latest results suggest both the reduction ability of the CuO by toluene and the amount of the oxygen vacancy determining the reaction rate.

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

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

Direct epoxidation of propylene with H_2 and O_2 to produce propylene oxide (PO), which could avoid the environmental and economic issues in the traditional processes, has received considerable attention since it was first reported over titania supported gold catalyst in 1998. Up to date, the low PO formation rate, low H_2 efficiency and poor catalysts stability still limit this route to realize commercialization. In this research, Au/TS-1 and Au/TiO_2 catalysts with different gold loading were prepared with deposition precipitation method. Catalytic performance test was performed in a fixed bed reactor with UV-vis to monitor the coordination states of Au and Ti sites, and MS to obtain the products distributions. H_2 and O_2 were used to produce hydrogen peroxide to oxidize Ti sites, and C_3H_6 was employed to reduce Ti-OOH species to finish the redox cycle. This could be used to determine the real oxidation states of Au and Ti sites and identify the rate determining step in the propylene epoxidation. On the other hand, in-situ FT-IR was used to probe the adsorbed species on the catalysts surface to investigate the coke formation mechanism. With these fundamental experimental data, it will be possible to have a better understanding of the reaction mechanism and thereby for better catalyst design and optimization.

Design of nitrogen-doped carbon materials for oxygen reduction reaction

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

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

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

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

To date, Fe-N-P-Cl- doped carbon spheres with high-N-content of 16.85 % and ultrahigh specific surface area of 1434 m^2/g are prepared successfully and applied as electrocatalysts for ORR in alkaline media. The E_{onset} (1.14 V vs. RHE) and E_{half} (0.86 V vs. RHE) are both higher than 30% Pt/C benchmark catalyst, confirming the good activity of the electrocatalyst. Based on the RRDE curves, the H_2O_2 yield is less that 2 % and the average electron transfer number is estimated to be 3.8, which is very close to 3.73−3.88 determined by RDE tests, slightly lower than that of 30% Pt/C (3.95). This suggests that the ORR catalysed by Fe-N-P-Cl- doped carbon spheres are carried out via an efficient four-electron pathway.

SINTEF projects

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

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)

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

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

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

The main objectives of 4REFINERY are:
To develop new biofuels production technology while at the same time increase understanding and control of the entire value chain
To scale up materials and testing procedures to define scenarios for the best further implementation in existing refineries
To develop solutions to answer key societal & environmental challenges
The project will focus on the transformation of bio-liquids from fast pyrolysis and hydrothermal liquefaction into advanced biofuels, through intermediate process steps combined with downstream co-processes technologies. The goal will be to bring these technologies from TRL3-4 to TRL4-5. The project will establish relations between product's properties, the quality of renewable feedstocks and all relevant process parameters along the value chain. The study of these combinations will allow a full understanding of the influence of feedstock and treatment processes on product characteristics.

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

Publications
[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-hydroprocessing of stabilized and deoxygenated pyrolysis oil fractions in rape seed oil and straight run gas oil, Submitted to Renewable Energy (Dec. 2020).

Biofuels from waste to road transport

(Waste2Road, 2018 – 2022)

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

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

Waste2Road will develop a new generation cost-effective biofuels from low cost and abundant biogenic residues and waste fractions. This will be achieved through optimization of European was recycling logistics and development of efficient conversion technologies, giving carbon yields > 45% with greenhouse gas (GHG) savings > 80%. The consortium will deploy risk-mitigation pathways to realis industrial implementation, with primary processing at European waste recycling sites and co-processing within European refineries. SINTEF will study catalytic hydrotreating and co-hydrotreating (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.

FISCHER-TROPSCH CATALYST SCREENING

Project category: Industry project

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

The objective of the project was improved understanding of Velocys' reactors by measuring the FT performance of spent F-T catalysts.

Client: VELOCYS

Philosophiae Doctor (PhD) theses in 2020

Xiaoyang Guo – Tuesday, 23 June
Inhibiting carbon growth at the initial stage of metal dusting corrosion of high temperature alloys
Public trial lecture: Gaseous reduction of metal oxides – in particular iron oxides

Opponent Professor Christian Hulteberg, Lund University.

Opponent: Dr. Anette Nørgaard, Haldor Topsøe, Denmark

Administrator: Professor Leif Kolbeinsen, NTNU

Main super visor: Professor Hilde Venvik, Xiaoyong Guo

Celebrations

Master (Diploma) Students in 2020

Ingvill Andrea Røed; *Low temperature selective hydrogenation using noble metal catalysts*

Petter Tingelstad; *Biomass conversion to fuels / Oxidation, autoclave, catalyst*

Kishore Rajendran; *Biomass conversion to chemical/Fixed bed reactor, ethanol*

Oscar Ivanez Encinas; *High temperature CO2 capture/combustion – fixed bed*

Maren Wasasås Kveinå; *CO2 emission reduction by CO to carbon/CNF – fixed bed*

Yun Liu; *Low temperature CO2 capture /TGA*

Jithin Gupakumar; *Ethylene oxychlorination on Cu based catalysts*

Hammad Farooq; *Carbon formation and catalysis in the conversion of methyl chloride and silicon into dimethyldichlorosilane*

Jørgen Lausund Grinna; *Low temperature CO2 capture by solid sorbents*

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

Susanne Klungland Stokkevåg; *Oxidation of methanol to formaldehyde (MTF) over Ag catalysts*

Anne Charlotte Gufsre Wold; *Kinetic study of process for high temperature CO2 capture by solid sorbents*

Jon Arve Selnes; *Catalytic methane abatement for natural gas engines*

Erik Søreide Hansen; *Hydrogen production from biomass derived compounds by sorption enhanced reforming*

Julie Christine Claussen; *Polymers Assisted Preparation of Iron based Fischer-Tropsch Catalsts for biomass to fuel/ Oxidation autoclave catalysts*

Exchange Bachelor Students in 2020

Philip Walter Putze*; Methodology Development for the Characterisation of Contact Mass in the Direct Process*

Rodrigo Ortiz Sánchez-Ramos; *Pelletized shaped Mn-based solid-sorbents for chemical looping desulfurization*

Group meetings 2020

KinCat

Catalysis Group – SINTEF – NTNU

Group meetings with seminars
Catalysis Group, Spring 2020

Location: Room K5- 428/429 and Webinars

Schedule	Time	Presenter	Topic
January 30	14:00	Marie Døvre Strømsheim	Investigations of the surface dynamics of Pd-alloy surfaces under oxidation reactions
February 8	14:00	Ole H. Bjørkedal	One Pot Synthesis of Highly Dispersed Mesoporous Fe and Cu Catalysts for NH$_3$ -SCR
April 17	14:00	Kjell Molljord	Low Carbon Transportation Fuels
May 8	14.00	Kumar Ranjan Rout	Biomass to Aviation Fuel through fast hydro pyrolysis integrated with catalytic upgrading
May 29	14:00	Moses Mawanga	O$_2$ -activation dictates NO to NO$_2$ Oxidation Catalysis

KinCat

Catalysis Group – SINTEF – NTNU

Group meetings with seminars
Catalysis Group, Fall 2020

Location: Room K5- 428/429

Schedule	Time	Presenter	Topic
September 4	14:00	Hongfei Ma	Ethylene oxychlorination for VCM production.
September 18	14:00	Ole H. Bjørkedal	One Pot Synthesis of Highly Dispersed Mesoporous Fe and Cu Catalysts for NH$_3$.
October 2	14:00	Marie Døvre Strømsheim	Investigations of the surface dynamics of Pd-alloy surfaces under oxidation reactions.
October 16	14.00	Alessandra Beretta iCSI -Seminar	Postponed
October 30	14:00	Alessandra Beretta	NH$_3$_SCR over V-based catalysts: Kinetic investigation on the role of NO+O$_2$ in the reduction steps of V redox cycle.
November 13	14:00	Rune Lødeng	Electrification, the premise of zero-emission and sustainability. A different story.
November 27	14:00	Wei Zhang	Size Dependence of Pt Catalysts for Propane Dehydrogenation: from Atomically Dispersed to Nanoparticles.
December 11	14:00	Ask Lysne	Catalytic Steam Reforming of Hydrocarbon Impurities from Biomass Gasification

Courses given by Group Members

TKP4110 Chemical Reaction Engineering

Coordinator: Professor De Chen

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

Semester: Fall

Level: 3th year

Credits: 7.5 SP

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

Objectives:

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

Prerequisites:

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

Contents:

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

Learning methods and activities:

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

Course material:

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

Exam: Written + exercises

TKP4150 Industrial Chemistry and Refining

Responsible: Professor Edd A. Blekkan

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

Semester: Spring

Level: 4th year.

Credits: 7.5 SP

Restricted Admission: No

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

Objectives:

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

Prerequisites:

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

Contents:

Feedstocks, Norwegian oil and gas production, energy from fossil fuels. Oil refining, oil products, refinery design and selected processes, catalytic reforming and isomerization, hydrotreating and hydrocracking, catalytic cracking, treatment of heavy oils, environmental concerns, new fuels. Examples of basic, intermediate and end products from petrochemistry. Natural gas and LPG as feedstock, synthesis gas production, preparation and use of hydrogen, methanol synthesis, Fischer-Tropsch, ammonia synthesis. Production of light olefins by steam-cracking, dehydrogenation and other routes, use of light olefins. Brief introduction to biomass as the feedstock for biofuels and chemicals, carbon capture and utilization (CCU).

Learning methods and activities:

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

Course material:

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

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

Exam: Written

TKP4155 Reaction Kinetics and Catalysis

Responsible: Professor Magnus Rønning

Lecturer: Professor Magnus Rønning

Semester: Fall

Level: 4th year

Credits: 7.5 SP

Restricted Admission: No

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

Objectives:

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

Prerequisites:

Course TKP4110 Chemical Reaction Engineering or similar knowledge.

Contents:

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

Learning methods and activities:

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

Course material:

I. Chorkendorff. J.W. Niemantsverdriet: Concepts of Modern Catalysis and Kinetics, Wiley-VCM.2007. 3^{rd} Edition

Exam: Written

TKP4190 - Fabrication and Applications of Nanomaterials

Responsible: Professor Jens-Petter Andreassen

Lecturers: Dr. Marie D. Strømsheim, Dr. Sulalit Bandyopadhyay, Dr. Seniz Ucar

Semester: Spring

Level: 3/4th year.

Credits: 7.5 SP

Restricted Admission: No

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

Objective:

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

Prerequisites:

Basis chemistry and mathematics and course TMT4320 Nanomaterials.

Contents:

The course starts by deriving the thermodynamic driving force and the kinetics of nucleation and growth of nanoparticles by focusing on precipitation from solutions. Different mechanism for nucleation and crystal growth along with calculations of nucleation and growth rates define the basis for design of different particle populations. The classical crystallization theory is presented as the fundamental theoretical background and recently emerging alternative hypotheses are discussed.

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

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

Learning methods and activities:

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

Catalysis and petrochemistry MSc specialization

Coordinator: Professor Edd Anders Blekkan

The specialization involves the following courses:

TKP4580 - Catalysis and Petrochemistry, Specialization Project	15 SP
TKP4581 - Catalysis and Petrochemistry, Specialization Project	7.5 SP
TKP4515 - Catalysis, Specialization Course	7.5 SP

TKP4580/81 Catalysis and Petrochemistry, Specialization Project

Semester: Normally fall, adjustments in special cases

Level: 5th year.

Credits: 7.5 SP

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

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

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

Prerequisites: None

Course description:

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

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

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

Course material: Handouts

TKP4515 - Catalysis, Specialization Course

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

- Environmental catalysis - (3.75 SP).

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

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

Semester: Fall

Level: 5th year.

Credits: 7.5 SP

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

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

Course material: Handouts, Papers and Chapters from textbooks.

Language: English

Module 1 - Environmental and energy catalysis

Responsible: Professor Hilde J. Venvik

Module description:

Catalysis occupies an important position within areas such as environmental technology and energy production. Within environmental technology catalysis has become crucial not only for removing of unwanted components such as NO_X, sulfur etc., but also for the development of selective processes. The course will give the fundamentals for catalytic processes for purification of exhaust gases (NO_X, CO, unburned hydrocarbons etc.). Within energy production the focus is on biofuel production, catalytic combustion, production of H_2 and catalysis/reactor technology related to fuel cells. Catalysis for clean production is also included to the course. At the end of the course the students should be able to describe important applications of heterogeneous catalysts in energy conversion, emissions clean-up, and clean production.

Module 2 Heterogeneous catalysis, advanced course

Responsible: Professor Edd Anders Blekkan

Module description:

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

Ph.D. courses

KP8132 Applied heterogeneous catalysis

Responsible: Professor Hilde Venvik

Credits: 7.5 SP

Prerequisites: TKP4155 Reaction kinetics and catalysis.

Course description:

The course is given every second year, next time in the fall term 2021.

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.

Course description:

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 2020

1. Gavrilovic, Ljubisa; Jørgensen, Erik Andreas; Pandey, Umesh; Putta, Koteswara Rao; Rout, Kumar Ranjan; Rytter, Erling; Hillestad, Magne; Blekkan, Edd Anders. Fischer-Tropsch synthesis over an alumina-supported cobalt catalyst in a fixed bed reactor – Effect of process parameters. Catalysis Today 2020. https://doi.org/10.1016/j.cattod.2020.07.055
2. Ma, Jianyu; Rout, Kumar Ranjan; Sauer, Maximilian; Mahmoodinia, Mehdi; Blekkan, Edd Anders. Investigations of molybdenum-promoted manganese-based solid sorbents for H_2S capture. Biomass & Bioenergy 2020 ;Volum 143. https://doi.org/10.1016/j.biombioe.2020.105843
3. Bjørkan, Hilde; Rønning, Magnus; Venvik, Hilde Johnsen; Johannessen, Tue; Holmen, Anders. Water–Gas Shift Activity of Pt Catalysts Prepared by Different Methods. Catalysts 2020 ;Volum 10 (10) s. 1132
4. Hjorth, Ida; Wang, Yalan; Li, Yahao; Buan, Marthe Emelie Melandsø; Nord, Magnus Kristofer; Rønning, Magnus; Yang, Jia; Chen, De. Electrochemical syngas production from CO_2 and water with CNT supported ZnO catalysts. Catalysis Today 2020 ;Volum 357. s. 311-321
5. Swirk, Katarzyna; Zhang, Hailong; Li, Shanshan; Chen, Yaoqiang; Rønning, Magnus; Motak, Monika; Grzybek, Teresa; Da Costa, Patrick. Carbon-resistant NiO-Y_2O_3-nanostructured catalysts derived from double-layered hydroxides for dry reforming of methane. Catalysis Today 2020 s. 1-11
6. Świrk, Katarzyna; Rønning, Magnus; Motak, Monika; Grzybek, Teresa; Da Costa, Patrick.Synthesis strategies of Zr- and Y-promoted mixed oxides derived from double-layered hydroxides for syngas production via dry reforming of methane. International Journal of Hydrogen Energy 2020 s. -
7. Zubair, Muhammad; Svenum, Ingeborg-Helene; Rønning, Magnus; Yang, Jia. Core-Shell Nanostructures of Graphene-Wrapped CdS Nanoparticles and TiO_2 (CdS@G@TiO_2): The Role of Graphene in Enhanced Photocatalytic H_2 Generation. Catalysts 2020 ;Volum 10.(4) s. –
8. Zubair, Muhammad; Vanhaecke, Estelle Marie M.; Svenum, Ingeborg-Helene; Rønning, Magnus; Yang, Jia. Core-shell particles of C-doped CdS and graphene: A noble metal-free approach for efficient photocatalytic H_2 generation. Green Energy & Environment 2020 ;Volum 5.(4) s. 461-472
9. 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 2020 s. 1-14
10. Strømsheim, Marie Døvre; Svenum, Ingeborg-Helene; Farstad, Mari Helene; Weststrate, C. J.; Borg, Anne; Venvik, Hilde Johnsen. CO-Induced Surface

Reconstruction of the Co(11–20) Surface—A Combined Theoretical and Experimental Investigation. Journal of Physical Chemistry C 2020 ;Volum 124.(52) s. 28488-28499

11. Svenum, Ingeborg-Helene; Herron, Jeffrey A.; Mavrikakis, Manos; Venvik, Hilde Johnsen. Pd3Ag(111) as a Model System for Hydrogen Separation Membranes: Combined Effects of CO Adsorption and Surface Termination on the Activation of Molecular Hydrogen. Topics in catalysis 2020 ;Volum 63. s. 750-761
12. Du, Juan; Kang, Le; Zhong, Qifan; Zhou, Haitao; Yang, Jianhong; Chen, De; Luo, Yingtao; Chen, Kaibin; Li, Wangxing; Xiao, Jin .High Peel Strength and Flexible Aligned Carbon Nanotubes/Etched Al Foil Composites with Boosted Supercapacitor and Thermal Dissipation Performances. Industrial & Engineering Chemistry Research 2020 ;Volum 59.(4) s. 1549-1558
13. Gao, Hongquan; Zhang, Dong; Zhou, Haitao; Wu, Jianchun; Xu, Guijiang; Huang, Zengliang; Liu, Menghao; Yang, Jianhong; Chen, De. Boosting Gravimetric and Volumetric Energy Density of Supercapacitors by 3D Pomegranate-like Porous Carbon Structure Design. Applied Surface Science 2020 ;Volum 534.
14. Hjorth, Ida; Wang, Yalan; Li, Yahao; Buan, Marthe Emelie Melandsø; Nord, Magnus Kristofer; Rønning, Magnus; Yang, Jia; Chen, De. Electrochemical syngas production from CO_2 and water with CNT supported ZnO catalysts. Catalysis Today 2020 ;Volum 357. s. 311-321
15. Rytter, Erling; Yang, Jia; Borg, Øyvind; Holmen, Anders. Significance of C_3 Olefin to Paraffin Ratio in Cobalt Fischer–Tropsch Synthesis. Catalysts 2020 ;Volum 10. s. 967
16. Wang, Yalan; Xiao, Ling; Qi, Yanying; Yang, Jia; Zhu, Yi-An; Chen, De. Insight into Size- and Metal-Dependent Activity and the Mechanism for Steam Methane Re-forming in Nanocatalysis. Journal of Physical Chemistry C 2020 ;Volum 124. s. 2501-2512
17. Yang, Jia; Rodriguez, Cristian Ledesma; Qi, Yanying; Ma, Hongfei; Holmen, Anders; Chen, De. The effect of co-feeding ethene on Fischer-Tropsch synthesis to olefins over Co-based catalysts. Applied Catalysis A : General 2020 ;Volum 598. s. 117564
18. Yang, Xiaoli; Wang, Ruifeng; Yang, Jia; Qian, Weixin; Zhang, Yaru; Li, Xuning; Huang, Yanqiang; Zhang, Tao; Chen, De. Exploring the Reaction Paths in the Consecutive Fe-Based FT Catalyst–Zeolite Process for Syngas Conversion. ACS Catalysis 2020 ;Volum 10.(6) s. 3797-3806
19. Zhou, Haitao; Liu, Menghao; Gao, Hongquan; Hou, Dong; Yu, Chongchen; Liu, Chao; Zhang, Dong; Wu, Jian-Chun; Yang, Jianhong; Chen, De. Dense integration of solvent-free electrodes for Li-ion supercabattery with boosted low temperature performance. Journal of Power Sources 2020 ;Volum 473. s. 1-9

20. Zubair, Muhammad; Svenum, Ingeborg-Helene; Rønning, Magnus; Yang, Jia. Core-Shell Nanostructures of Graphene-Wrapped CdS Nanoparticles and TiO2 (CdS@G@TiO2): The Role of Graphene in Enhanced Photocatalytic H2 Generation. Catalysts 2020 ;Volum 10.(4) s. –
21. Zubair, Muhammad; Vanhaecke, Estelle Marie M.; Svenum, Ingeborg-Helene; Rønning, Magnus; Yang, Jia. Core-shell particles of C-doped CdS and graphene: A noble metal-free approach for efficient photocatalytic H2 generation. Green Energy & Environment 2020 ;Volum 5.(4) s. 461-472
22. Chang, Hui; Bjørgum, Erlend; Mihai, Oana; Yang, Jie; Lein, Hilde Lea; Grande, Tor; Raaen, Steinar; Zhu, Yi-an; Holmen, Anders; Chen, De. Effects of Oxygen Mobility in La-Fe-Based Perovskites on the Catalytic Activity and Selectivity of Methane Oxidation. ACS Catalysis 2020 ;Volum 10.(6) s. 3707-3719
23. Niu, Juntian; Wang, Yalan; Qi, Yanying; Dam, Anh Hoang; Wang, Hongmin; Zhu, Yi-An; Holmen, Anders; Ran, Jingyu; Chen, De. New mechanism insights into methane steam reforming on Pt/Ni from DFT and experimental kinetic study. Fuel 2020 ;Volum 266. s. 1-12
24. Yang, Jia; Rodriguez, Cristian Ledesma; Qi, Yanying; Ma, Hongfei; Holmen, Anders; Chen, De. The effect of co-feeding ethene on Fischer-Tropsch synthesis to olefins over Co-based catalysts. Applied Catalysis A : General 2020 ;Volum 598. s. -
25. Acha, E; Chen, De; Cambra, J. Comparison of novel olivine supported catalysts for high purity hydrogen production by CO2 sorption enhanced steam reforming. Journal of CO2 Utilization 2020 ;Volum 42. s. 1-14
26. Capa, Alma; García, Roberto; Chen, De; Rubiera, Fernando; Pevida, Covadonga; Gil, Mara Victoria. On the effect of biogas composition on the H2 production by sorption enhanced steam reforming (SESR). Renewable Energy 2020 ;Volum 160. s. 575-583
27. Chang, Qing-Yu; Wang, Kai-Qi; Hu, Ping; Sui, Zhi jun; Zhou, Xinggui; Chen, De; Yuan, Wei-kang; Zhu, Yi-an.Dual-Function Catalysis in Propane Dehydrogenation over Pt1–Ga2o3 Catalyst: Insights from a Microkinetic Analysis.. AIChE Journal 2020 ;Volum 66.
28. Chang, Qing-Yu; Wang, Kai-Qi; Hu, Ping; Sui, Zhi-Jun; Zhou, Xing-Gui; Chen, De; Yuan, Wei-Kang; Zhu, Yi-An. Dual-function catalysis in propane dehydrogenation over Pt1-Ga2O3 catalyst: Insights from a microkinetic analysis. AIChE Journal 2020 ;Volum 66.(7) s. –
29. Chen, Qingjun; Wang, Siyu; Rout, Kumar Ranjan; Chen, De. Development of Polyethylenimine (PEI)-impregnated mesoporous carbon spheres for low-concentration CO2 capture. Catalysis Today 2020 s. -
30. Chen, Wenyao; Chen, Shuangming; Qian, Gang; Song, Li; Chen, De; Zhou, Xinggui; Duan, Xuezhi. On the nature of Pt-carbon interactions for enhanced hydrogen generation. Journal of Catalysis 2020 ;Volum 389. s. 492-501

31. Chen, Wenyao; Fu, Wenzhao; Chen, Bingxu; Peng, Chong; Qian, Gang; Chen, De; Duan, Xuezhi; Zhou, Xinggui.Polymer decoration of carbon support to boost Pt-catalyzed hydrogen generation activity and durability. Journal of Catalysis 2020 ;Volum 385. s. 289-299
32. Chen, Wenyao; Fu, Wenzhao; Qian, Gang; Zhang, Bingsen; Chen, De; Duan, Xuezhi; Zhou, Xinggui. Synergistic Pt-WO3 Dual Active Sites to Boost Hydrogen Production from Ammonia Borane. iScience 2020 ;Volum 23.(3) s. 1-13
33. Chen, Wenyao; Zheng, Weizhong; Cao, Junbo; Fu, Wenzhao; Qian, Gang; Chen, De; Zhou, Xinggui; Duan, Xuezhi. Atomic Insights into Robust Pt-PdO Interfacial Site-Boosted Hydrogen Generation. ACS Catalysis 2020 ;Volum 10.(19) s. 11417-11429
34. Du, Juan; Kang, Le; Zhong, Qifan; Zhou, Haitao; Yang, Jianhong; Chen, De; Luo, Yingtao; Chen, Kaibin; Li, Wangxing; Xiao, Jin.High Peel Strength and Flexible Aligned Carbon Nanotubes/Etched Al Foil Composites with Boosted Supercapacitor and Thermal Dissipation Performances. Industrial & Engineering Chemistry Research 2020 ;Volum 59.(4) s. 1549-1558
35. Fenes, Endre; Qi, Yanying; Ma, Hongfei; Zhu, Jun; Wang, Yalan; Rout, Kumar Ranjan; Fuglerud, Terje; Piccinini, Marco; Chen, De. Prediction and Tuning of the Defects in the Redox Catalysts: Ethylene Oxychlorination. ChemCatChem 2020 ;Volum 13. s. 221-226
36. Gao, Hongquan; Zhang, Dong; Zhou, Haitao; Wu, Jianchun; Xu, Guijiang; Huang, Zengliang; Liu, Menghao; Yang, Jianhong; Chen, De. Boosting Gravimetric and Volumetric Energy Density of Supercapacitors by 3D Pomegranate-like Porous Carbon Structure Design. Applied Surface Science 2020 ;Volum 534.
37. Guan,, Y.; Ma,, H.; Chen,, W; Li,, M.; Qian, Gang; Chen, De; Zhou, Xinggui; Duan, Xuezhi. Methyl Methacrylate Synthesis: Thermodynamic Analysis for Oxidative Esterification of Methacrolein and Aldol Condensation of Methyl Acetate. Industrial & Engineering Chemistry Research 2020 ;Volum 59. s. 17408-17416
38. 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 2020 s. 1-14
39. Hjorth, Ida; Wang, Yalan; Li, Yahao; Buan, Marthe Emelie Melandsø; Nord, Magnus Kristofer; Rønning, Magnus; Yang, Jia; Chen, De. Electrochemical syngas production from CO2 and water with CNT supported ZnO catalysts. Catalysis Today 2020 ;Volum 357. s. 311-321

40. Lin, Dong; Zheng, Xiuhui; Feng, Xiang; Sheng, Nan; Song, Zhaoning; Liu, Yibin; Chen, Xiaobo; Cai, Zhenping; Chen, De; Yang, Chaohe. Enhancing the dynamic electron transfer of Au species on wormhole-like TS-1 for boosting propene epoxidation performance with H2 and O2. Green Energy & Environment 2020 ;Volum 5.(4) s. 433-443
41. Ma, Fang; Chang, Qing-Yu; Yin, Qiang; Sui, Zhi-Jun; Zhou, Xinggui; Chen, De; Zhu, Yi-An. Rational screening of single-atom-doped ZnO catalysts for propane dehydrogenation from microkinetic analysis. Catalysis Science & Technology 2020 ;Volum 10.(15) s. 4938-4951
42. Ma, Hongfei; Fenes, Endre; Qi, Yanying; Wang, Yalan; Rout, Kumar Ranjan; Fuglerud, Terje; Chen, De. Understanding of K and Mg co-promoter effect in ethylene oxychlorination by operando UV–vis-NIR spectroscopy. Catalysis Today 2020 s. -
43. Ma, Hongfei; Ma, Guoyan; Qi, Yanying; Wang, Yalan; Chen, Qingjun; Rout, Kumar Ranjan; Fuglerud, Terje; Chen, De. Nitrogen-Doped Carbon-Assisted One-pot Tandem Reaction for Vinyl Chloride Production via Ethylene Oxychlorination. Angewandte Chemie International Edition 2020 ;Volum 59.(1) s. 22080-22085
44. Ma, Hongfei; Sollund, Erling Olav; Zhang, Wei; Fenes, Endre; Qi, Yanying; Wang, Yalan; Rout, Kumar Ranjan; Fuglerud, Terje; Piccinini, Marco; Chen, De. Kinetic modeling of dynamic changing active sites in a Mars-van Krevelen type reaction: Ethylene oxychlorination on K-doped $CuCl_2/Al_2O_3$. Chemical Engineering Journal 2020 ;Volum 407. s. 1-10
45. Ma, Hongfei; Wang, Yalan; Qi, Yanying; Rout, Kumar Ranjan; Chen, De. Critical review of catalysis for ethylene oxychlorination. ACS Catalysis 2020 ;Volum 10.(16) s. 9299-9319
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49. Noor, Tayyaba; Qi, Yanying; Chen, De. Hydrogen dependence of the reaction mechanism and kinetics of water gas shift reaction on Ni catalyst: Experimental and DFT study. Applied Catalysis B: Environmental 2020 ;Volum 264. s. -
50. Qi, Yanying; Fenes, Endre; Ma, Hongfei; Wang, Yalan; Rout, Kumar Ranjan; Fuglerud, Terje; Marco, Piccinini; Chen, De. Cluster-size-dependent interaction

between ethylene and CuCl2 clusters supported via γ-alumina. Journal of Physical Chemistry C 2020 ;Volum 124. s. 10430-10440

51. Qi, Yanying; Fenes, Endre; Ma, Hongfei; Wang, Yalan; Rout, Kumar Ranjan; Fuglerud, Terje; Marco, Piccinini; Chen, De. Origin of potassium promotion effects on CuCl2/gamma-Al2O3 catalyzed ethylene oxychlorination. Applied Surface Science 2020 ;Volum 521. s. 1-9
52. Song, Zhaoning; Yuan, Juncong; Cai, Zhenping; Lin, Dong; Feng, Xiang; Sheng, Nan; Liu, Yibin; Chen, Xiaobo; Jin, Xin; Chen, De; Yang, Chaohe. Engineering Three-Layer Core–Shell S-1/Ts-1@ Dendritic-Sio2 Supported Au Catalysts Towards Improved Performance for Propene Epoxidation with H2 and O2.. Green Energy & Environment 2020 ;Volum 5.(4) s. 473-483
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55. Yalan Wang, Hongmin Wang, Anh Hoang Dam, Qi Ling, Yanying Qi, Junatian Niu, Jia Yang, Yi-An Zhu, Anders Holmen, De Chen: Understanding effects of Ni particle size on steam methane reforming activity by combined experimental and theoretical analysis, Catal. Today 355 (2020) 139-147
56. Hamidreza Bakhtiary-Davijany, Fatemeh Hayer, Xuyen Kim Phan, Rune Myrstad, Hilde Venvik, Peter Pfeifer, Anders Holmen: Modelling and simulation of a single slit micro packed bed reactor for methanol synthesis. Catal. Today 343 (2020) 226-233

Presentations in 2020

1. Blekkan, Edd Anders: CCU – en klimaløsning? Prosess 21 web-møte " Utnyttelse av karbon fra prosessgass (CCU). Muligheter for norsk prosessindustri "; 2020-05-20 - 2020-05-20
2. Blekkan, Edd Anders; Yang, Jia: Kinetics of NO oxidation over Pt and Mn Catalysts (A prologue to Intrinsic Transient NO oxidation Kinetics). iCSI Annual Seminar; 2020-09-15 - 2020-09-16
3. Lysne, Ask; Rout, Kumar Ranjan; Blekkan, Edd Anders: Catalytic Steam Reforming of Hydrocarbon Impurities from Biomass Gasification - Group meeting. NTNU Catalysis Group Meeting (Webinar); 2020-12-11 - 2020-12-11
4. Lysne, Ask; Rout, Kumar Ranjan; Blekkan, Edd Anders: Reforming of Hydrocarbon Impurities from Biomass Gasification. Bio4Fuels Days 2020: Working towards a climate-neutral 2050; 2020-11-18 - 2020-11-19
5. Mahmoodinia, Mehdi; Ma, Jianyu; Sauer, Maximilian; Rout, Kumar Ranjan; Blekkan, Edd Anders: Performance of Manganese-based Solid Sorbents for H2S Removal: Role of Particle Size and Promoter. 2020 iCSI annual seminar; 2020-09-14 - 2020-09-01
6. Yang, Jia; Blekkan, Edd Anders: Insights into the Reaction Mechanism and Kinetics of Industrial Catalyzed Reactions. iCSI Annual Seminar; 2020-09-15 - 2020-09-16
7. Bjørkedal, Ole Håvik; Regli, Samuel K.; Rønning, Magnus.One-Pot Synthesis of Highly Dispersed Mesoporous Fe and Cu Catalysts for NH3-SCR. International Conference on Environmental Catalysis; 2020-09-07 - 2020-09-09
8. Fenes, Endre; Ma, Hongfei; Rønning, Magnus; Rout, Kumar Ranjan; Chen, De; Fuglerud, Terje.Elucidating the copper species in alumina supported CuCl2-catalysts during oxychlorination of ethylene to 1,2-dichloroethane by operando XAFS, PXRD and UV-Vis using MCR-AR analysis. ESRF User Meeting 2020; 2020-02-03-2020-02-05
9. Regli, Samuel K.; Chen, De; Fenes, Endre; Rout, Kumar Ranjan; Ma, Hongfei; Fuglerud, Terje; Rønning, Magnus .Elucidating the copper species in alumina supported CuCl2-catalysts during oxychlorination of ethylene to 1,2-dichloroethane by operando XAFS, PXRD and UV-Vis using MCR-AR analysis. ESRF User Meeting 2020; 2020-02-03 - 2020-02-05
10. Regli, Samuel K.; Rønning, Magnus. Multivariate statistical analysis of in situ and operando X-ray Absorption Spectroscopy data. ESRF User Meeting, 2020-02-03 - 2020-02-05

11. Rønning, Magnus. Catalytic oxidation of NO to NO2 for nitric acid production. Catalysis Seminar, KYH, Stockholm, Sweden; 2020-02-28 - 2020-02-28
12. Strømsheim, Marie Døvre; Svenum, Ingeborg-Helene; Mahmoodinia, Mehdi; Boix, Virginia; Knudsen, Jan; Venvik, Hilde Johnsen. Investigations of the surface dynamics of Pd-alloy surfaces under oxidation reactions. International Conference on Environmental Catalysis 2020; 2020-09-07 - 2020-09-09

Seminars/Guest lectures/iCSI Seminars

iCSI has the pleasure of inviting you for a digital (Zoom) guest lecture given by **Professor Enrique Iglesia**, member of iCSI's Scientific advisory committee, on the topic **Redox Cycles in Oxidation Catalysis: C-H and O=O Activation Routes on Metal Oxides** Thursday June 18 at 15.00, European time.

iCSI has the pleasure of inviting you for a digital(Zoom) guest lecture given by **Professor Alessandra Beretta**, member of iCSI's Scientific advisory committe:
NH_3_SCR over V-based catalysts: Kinetic investigation on the role of NO+O_2 in the reduction steps of V redox cycle.
Friday October 30 at 14:00.

2020 iCSI Annual Seminar Program

Date: 14-15 September 2020.

Venue: Oscarsborg festning, Oslofjorden, close to Drøbak (35 min from Oslo, 65 min. from Oslo airport)

Day 0 (Sunday September 13)	
Afternoon:	**Board arrival and dinner**
Day 1 (Monday September 14)	
09:00-11:00	*Board meeting*
~11:00	Registration/check-in
11:30-12:30	**Lunch**
12:30-13:00	Opening remarks (Chair of the Board, Pablo Beato) Status of iCSI (Director, Hilde J. Venvik
13:00-14:00	IIA4 Achievements: PVC Value Chain: World class energy and raw material efficiency for production of Chlorine and Vinyl Chloride Monomer (VCM) Hongfei, Yalan, 20 min each, the rest for discussion
14:00-14:30	**Coffee break**
14:30-15:00	IIA2 Achievements: Abatement of nitrogen-containing pollutants. State-of-the-art catalyst technology Jasmina/Silje/Karl-Isak/David (15 min), the rest for discussion
15:00-16:00	IIA3 Achievements: Frontier formalin technology development Jasmina (5 min) Hilde (Stine), Roman/Kristin, Rune/Kristin 10 -15 min each, the rest for discussion
16:00-17:00	Break / New SFI meeting
17:00-18:00	**Poster session** with contributions from iCSI and related projects
18:00-20:00	**Break or social activity**
20:00-22:00	**Dinner**

Day 2 (Tuesday September 15)	
9:00-9:30	Presentation by Ingeborg-Helene Svenum: "Effect of promotors and inhibitors in Co-based FTS"
09:30-10:30	IIA5 Achievements: The next step in direct activation of lower alkanes Stian/Pablo/Karoline/Sebastian 30 min, the rest for discussion
10:30-11:00	**Coffee break**
11:00 - 12:10	IIA1 Achievements: 21st century Ammonia Oxidation and Nitric Acid technology development Anja (5min), Asbjørn/Julie (15 min), Silje (10 min), Magnus/Jithin (10 min), the rest for discussion
12:15-13:00	**Lunch**
13:00-14:10	IIA 6 Achievements: Generic projects for additional industrial synergies Magnus (Samuel) (15min), Oleksii (20 min), Moses (10 min), the rest for discussion
14:10	Closing remarks
14:45	**Departure Ferry to Drøbak or coffee (your choice 😎)**
15.45	**Departure Ferry to Drøbak**

Welcome!

The iCSI Management and administration team

Hilde & Anne

Trial Lectures for the PhD degree

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

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

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

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

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

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

Ola Olsvik: *Catalytic membrane reactors*. 1993

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

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

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

Geir Remo Fredriksen: Catalytic Combustion, 17/12 1993

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

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

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

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

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

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

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

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

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

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

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

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

Magnus Rønning: *Photocatalysis*. 2/3 2000

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

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

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

Lucie Bednarova: *Computational Catalysis*. 2002

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

Leiv Låte: *Catalysis in supercritical fluids*. 2002

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

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

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

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

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

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

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

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

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

Erlend Bjørgum: *Photocatalysis* 20/1 2006

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

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

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

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

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

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

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

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

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

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

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

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

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

Sara Boullosa Eiras: *Catalysts and materials development in solid oxide fuel cells*. 22/10 2010

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Ata ul Rauf Salman*: Nitrogen fixation beyond Haber-Bosch - recent developments in heterogeneous catalysis and electrocatalysis*. 6/12 2019

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

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

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

Xiaoyang Guo: *Gaseous reduction of metal oxides – in particular iron oxides 23/6 2020*

Alumni - PhD students Catalysis group:

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

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

Dag Schanke
Hydrogenation of CO over supported iron catalysts.
Defense of thesis: October 1986
Current position: Retired from Equinor, Trondheim.

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

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

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

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

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

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

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

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

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

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

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

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

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

Karina Heitnes Hofstad
Catalytic oxidation of methane to synthesis gas
Defense of thesis: 1996
Current position: Equinor.

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

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

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

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

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

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

Ketil Firing Hanssen
Cobalt Fischer-Tropsch catalysts studied by steady-state and transient kinetic methods
Defense of thesis: 1999
Current position: Senior engineer, DNV GL.

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

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

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

Thomas Sperle
Steam reforming of hydrocarbons to synthesis gas.
Defense of thesis: October 2001.
Current position: CoFounder AS, Trondheim.

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

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

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

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

Bozena Silberova
Oxidative dehydrogenation of ethane and propane at short contact time.
Defense of thesis: January 2003
Current position: Kuiper & Burger Advies- en Ingenieursbureau, Netherlands.

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

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

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

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

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

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

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

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

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

Florian Huber
Nanocrystalline copper-based mixed oxide catalysts for water-gas shift

Defense of thesis: August 2006
Current position: HTE, Germany.

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

Espen Standal Wangen
Characterisation and pyrolysis of heavy oils
Defense of thesis: May 2007
Current position: Teacher, Charlottenlund ungdomsskole, Trondheim.

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

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

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

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

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

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

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

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

Li He
Sorption enhanced steam reforming of biomass derived compounds
Defense of thesis: January 2010
Current position: Post.doc. NTNU

Sara Boullosa Eiras
Comparative study of selected catalysts for methane partial oxidation.
Defense of thesis: October 2010
Current position: Yara, Porsgrunn

Hamidreza Bakhtiary
Performance assessment of a packed bed microstructured reactor – heat exchanger for methanol synthesis from syngas.
Defense of thesis: November 2010
Current position: Xodus Group, Oslo

Xuyen Kim Phan
Catalyst formulations for use in microstructured reactors for conversion of synthesis gas to liquids.
Defense of thesis: January 2011
Current position: WellChem AS.

Fatemeh Hayer
Direct Synthesis of Dimethyl Ether in Microstructured Reactors
Defense of thesis: March 15 2011.
Current position: Aibel, Stavanger.

Shreyas Panduran Rane
Relation between Catalyst Properties and Selectivity in Fischer-Tropsch Synthesis
Defense of thesis: May 2011

Fan Huang
3D Carbon/polyaniline Nanostructures for Energy Storage
Defense of thesis: August 2011
Current position: Haliburton, Stavanger.

Oana Mihai
Partial Oxidation of Methane by Chemical Looping
Defense of thesis: September 2011
Current position: Post.doc. Chalmers, Sweden.

Jia Yang
A steady-State Isotopic Transient Kinetic Study of Cobalt Catalysts: Mechanistic Insights and Effect of Cobalt Particle Size, Supports and Promoters.
Defense of thesis: October 2011
Current position: Assoc. Professor, NTNU.

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

Kazi Saima Sultana
Calcium Based CO_2 Acceptors for Sorption Enhanced Steam Methane Reforming
Defense of thesis: November 2011.

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

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

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

Paul Radstake
Dehydrogenation of Ethane over Alumina-Supported Pt-Sn Catalysts
Defense of thesis: December 2012
Current position: Franzefoss Minerals, Hylla.

Ilya Viktorovich Gorelkin:
Concepts and models of the catalytic dehydrogenation of propane. Defense of thesis: March 2013
Current position: Siemens, Trondheim.

Tayyaba Noor
Sorption Enhanced Water Gas Shift Reaction: Materials and Catalysis. Defense of thesis: June 2013
Current position: School of Chemical and Materials Engineering, SCME, NUST, Islamabad, Pakistan.

Ingvild Tronstad
Corrosion of Copper and Oxidation of Dielectric Liquids in High Voltage Transformers.
Defense of thesis: June 2013
Current position: NAMMO Raufoss.

Fengliu Lou
Aligned carbon nanotubes@manganese oxide coaxial arrays for lithium ion batteries.
Defense of thesis: September 2013
Current position: Beyonder AS, Stavanger.

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

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

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

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

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

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

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

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

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

Xuehang Wang
Porous carbon prepared by chemical activation for high-energy supercapacitors in ionic liquid electrolyte
Defense of thesis*:* Sept. 30 2016
Current position: Post.doc. Department of Materials Science

and Engineering and A. J. Drexel
Nanomaterials Institute, Drexel
University, Philadelphia , PA
19104
USA.

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

Ida Hjort
Catalysis for electrochemical conversion of CO2 in aqueous solutions
Defense of thesis: March 31 2017
Current position: NAMMO, Raufoss.

Marie Døvre Strømsheim
Co{11-20} and Pd3Au{100} single crystals as catalyst model system.
Defense of thesis: Dec. 13, 2017
Current position: Post.doc. NTNU.

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

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

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

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

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

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

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

Xiaoyang Guo
Inhibiting carbon growth at the intial stage of metal dusting corrosion of high temperature alloys
Defense of thesis: June 23rd, 2020
Current position: Post.Doc. NTNU