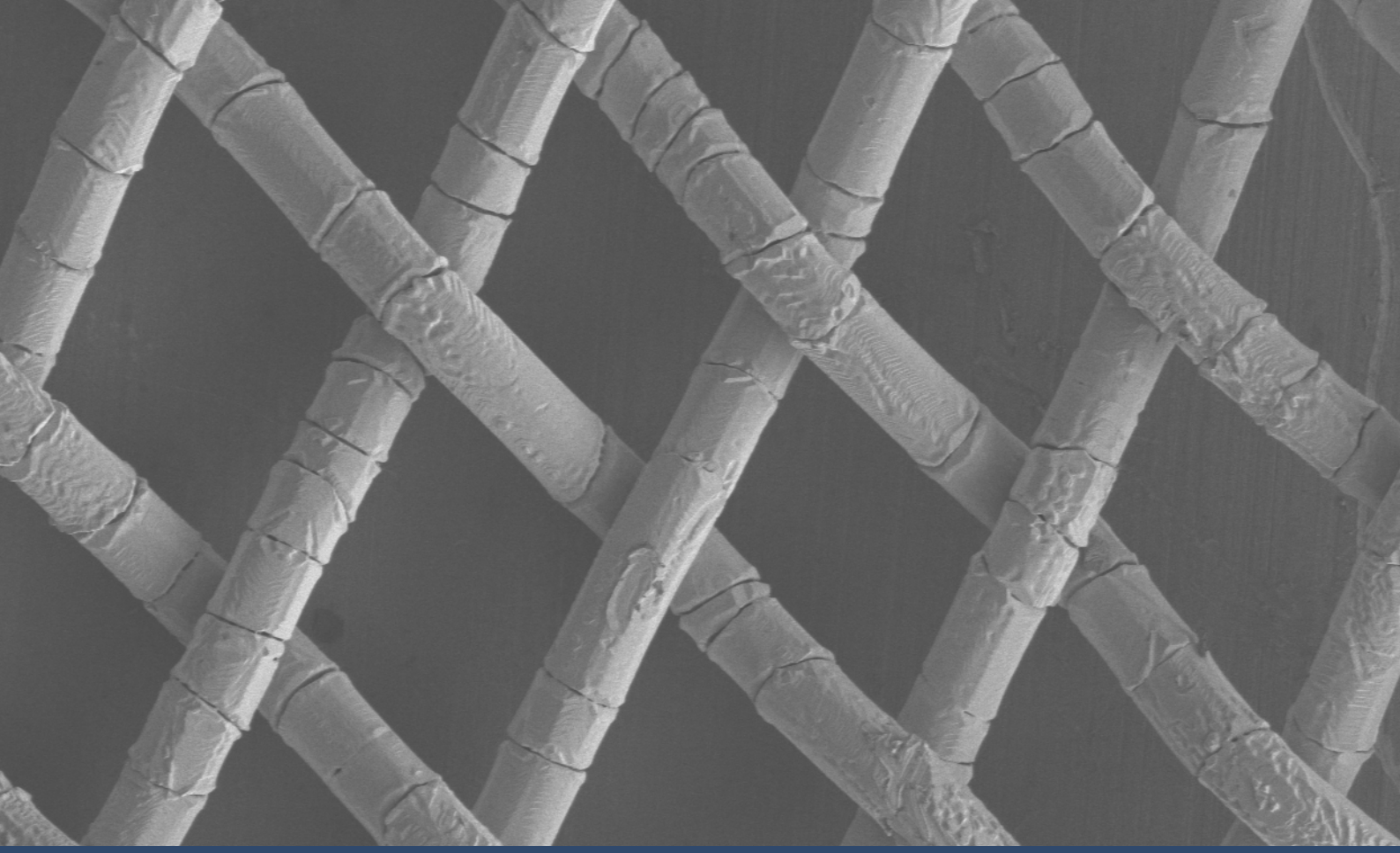


iCSI

industrial Catalysis Science and Innovation

Annual Report 2019

sfi Centre for Research-based Innovation

NTNU

iCSI Partners

Centre for Research-based Innovation

NTNU

UiO : Universitetet i Oslo

SINTEF

dynea

inovyn

HALDOR TOPSØE

YARA

K.A.Rasmussen Norway

The Research Council of Norway

Cover photo: *Pure Pd gauze annealed until the size of the grains exceeded the diameter of the wire and then exposed to Pt catchment. About 200 times magnification in scanning electron microscope (SEM) by Asbjørn Slagtern Fjellvåg. From IIA1 WP1.1.*

2019 Summary

2019 was a year of refreshing the iCSI Centre, with new people joining while others were leaving. First of all, we are proud of the first two iCSI PhDs, Dr. Ata ul Rauf Salman and Dr. Dimitrios Pappas, who both finalized their degrees in December. They are now in new positions in Norwegian industry, and we wish them success there. We have also welcomed two new PhD candidates to the University of Oslo, Karoline Kvande and Julie Hessevik, and a new Postdoctoral fellow to NTNU, Yalan Wang. All three are well qualified and motivated for their research tasks, and we look forward to following their work in the coming years.

Educating master's students is important to the Centre. In 2019, 13 master's students were associated with iCSI, of which five delivered directly into the ongoing projects. The gender balance within iCSI also improved this year, with all personnel categories now balancing – either way – within a 40/60 distribution.

In 2019 our young scientists and senior researchers continued to show their innovation potential by disseminating high quality research from the Centre. iCSI researchers gave 27 presentations at national and international conferences. The number of publications increased from the year before, and 18 reviewed papers were published. At the end of the year, even more were submitted for review. The publication and presentations lists can be found on p. 58-60.

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

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

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

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

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

Content

Time to refresh!

In many senses, the past year has been a time for refreshing the iCSI Centre! It is now 4 ½ years since the iCSI board was established and the last contract details of the iCSI consortium were finalized. Several personnel changes have occurred since then and in 2019, the composition of the Board was refreshed again. Torgeir Lunde, the representative from Yara, replaced Board chair Odd-Arne Lorentsen. UiO representative Einar Uggerud (Head of Chemical department) replaced Kristin Vinje, and Marco Piccinini, the representative from Inovyn, replaced Terje Fuglerud. I have been a member of the Board since its founding and when Odd-Arne left, the Board decided to appoint me as the new Chair. I am grateful for their confidence and it is a real pleasure to work with so many passionate and engaged people. In particular, I appreciate the collaboration with Hilde and Anne, who are not only the leaders but also the souls of the management group. They have navigated us effectively and successfully through the midway evaluation process, which is enabling us to continue the Centre's work for the next five years.

However, the workhorses of the Centre are of course the PhD students and postdoctoral fellows. In the beginning of 2016, we started to hire PhD students, and the scientific work at iCSI was launched. Now in 2019, we are proud to have witnessed the first iCSI students obtaining their PhD degree. Ata ul Rauf Salman defended his thesis, entitled Catalytic oxidation of NO to NO2 for nitric acid production on December 6, 2019. A week later, on December 13, 2019, Dimitrios Papas defended his thesis, entitled Direct methane to methanol conversion over Cu-exchanged zeolites: Building structure – activity relationships. As a co-supervisor of Dimitrios, it has been an amazing journey to follow his growth, both scientifically and personally. It is even more satisfying to know that both newly minted doctors have obtained positions in industry and are now part of the Norwegian labour market. Three PhD defences will follow in 2020 and, as is typical for mature scientific work, this correlates well with the steep increase in the number of scientific publications coming from the iCSI Centre during 2019. I am sure that this trend will continue through 2020 and beyond.

However, 2020 will also be a time to refresh the scene with the new PhD candidates and postdocs who started at the iCSI Centre during 2019: Karoline Kvande (PhD) at UiO/Topsøe, Julie Hessevik (PhD) at UiO/KA Rasmussen/Yara and Yalan Wang (postdoc) at NTNU/ Inovyn. Another five new young researchers will be hired this year, and it is comforting to know that they will find a well-functioning infrastructure, which further guarantees the progress in their respective innovation areas.

In my view, the start of the next cycle of students will also be a good opportunity for all of us to refresh our ideas. We have to sit down and try to learn from our scientific and personal experiences and listen to the advice given to us by the midway evaluation and our internal scientific advisory committee (SAC). In November 2019, we actually organized a leader meeting to do so – what better place could we have chosen than Farris Bad at a hotel under the motto "Relax, Rejuvenate, Refresh"!

In this sense, I hope that we constantly rethink or adjust our research goals and try to think "out of the box", thereby ensuring that we are still focusing on the right problems and making use of the unique possibility we have been given to create innovation within the iCSI Centre.

Pablo Beato

iCSI Board Chair

Vision, objectives and strategy

iCSI focuses on Catalysis Science and Innovation related to a range of industrial processes that are key to Norwegian land-based industry, industrial competitiveness, as well as future chemical processing and energy conversion with a minimum environmental footprint. The industrial partners involved supply key sectors of the global market (catalysts, chemicals, fertilizer, plastics, fuels, etc.), which are the very products that impact our food supply and standard of living the most. The iCSI consortium represents leading competence and technology, for which the core business relies largely or completely on catalytic processes. iCSI represents significant industrial operations in Norway as well as worldwide.

iCSI's basic vision has been to establish an integrated competence and technology platform that promotes world class energy and raw material efficiency and allows spin-off activities in the different directions of prime interest for the industrial partners. Furthermore, iCSI is developing a strong competence base for the Norwegian chemical industry in the long term and to the benefit of society in terms of securing jobs, reducing energy consumption and abating harmful emissions to the environment. State-of-the-art methodology in synthesis, characterization and technology development is applied in order to obtain a detailed understanding of complex catalysts under industrially relevant conditions, thereby identifying factors critical to their performance. iCSI researchers also develop predictive tools for optimization of materials, chemistries and processes.

Photo: Reidar Lunde Lillestøl

iCSI's main objective is to boost industrial innovation and competitiveness and provide efficient, low-emission processes.

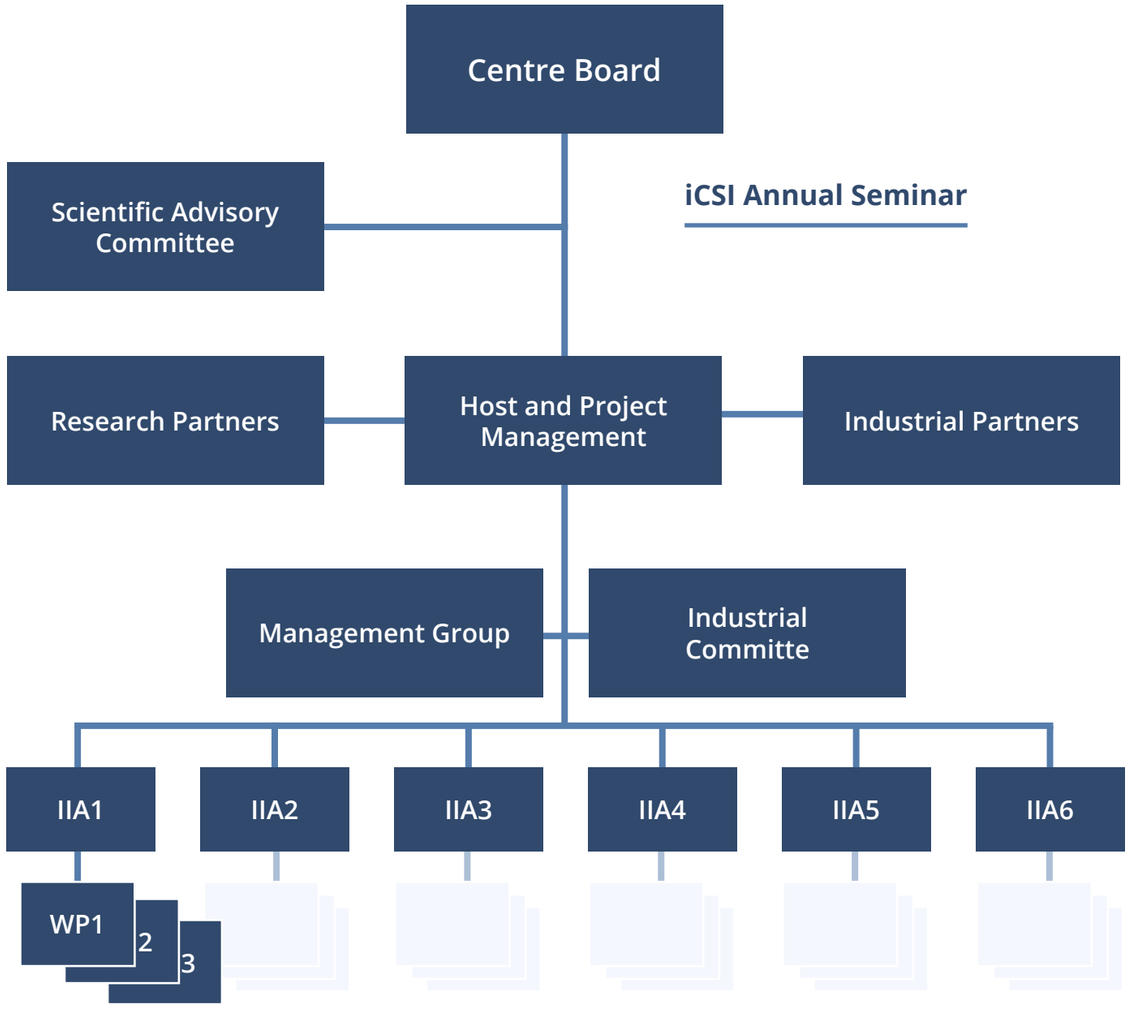
This can be achieved though:

- Improved understanding of the kinetics and chemistry of the catalytic processes as a basis for performance enhancement and process optimization.
- Synergy between applied and basic research, competence-building and education through interaction between industry, research institutes and universities
- Development of new materials and experimental and theoretical methods

iCSI organization

The Norwegian University of Science and Technology (NTNU) is serving as Host institution for the iCSI Centre. The iCSI research partners – NTNU, SINTEF Industry and the University of Oslo (UiO) – represent the main research groups involved in heterogeneous catalysis research in Norway, located in Trondheim (NTNU and SINTEF) and Oslo (UiO and SINTEF). The industrial partners – Yara, KA Rasmussen AS, Dynea, INOVYN and Haldor Topsøe A/S – also conduct their own significant R&D. The collaboration enables the optimized use of complementary competence and a shared, highly advanced, experimental infrastructure that is being utilized, expanded and developed within iCSI.

The research is organized into 6 Industrial Innovation Areas (IIA1-6), each with 1-6 work packages. Cutting-edge research topics addressing the key challenges are identified for each of the iCSI industrial innovation areas (IIA)1-5 and defined as Work Packages. IIA6 is focusing on the development of methodology in line with the international forefront, and these methods are gradually being integrated into the activities of IIA1-5. Each IIA has 2-3 research partners and 1-2 industrial partners, while IIA6 is generic and involves all partners.



Industrial Partners

An overall objective for iCSI is to strengthen the competitive position of the industrial partners by securing their technological lead with respect to selected catalysts and process operations and enabling them to further reduce their environmental footprint. In addition, certain Norwegian industrial operations and industrial core competences can be secured and developed.

Yara International ASA is a Norwegian-based chemical company with fertilizer as its largest business area. Yara also works with industrial gases, catalyst production and NOx abatement solutions for industrial plants, vehicles and vessels in its product portfolio. In addition to being present in more than 51 countries, Yara operates 2 industrial production sites in Norway, Porsgrunn and Glomfjord, with approx. 700 employees. In iCSI, Yara aims to further strengthen its global competitiveness through innovation.

KA Rasmussen AS is a refiner of precious metals and supplier of catalysts and products based on precious metals located in Hamar, Norway among other places in Europe. KA Rasmussen has specialized in technology for producing structured catalysts for the Ostwald process, and silver particles for the oxidation of methanol. In iCSI, KA Rasmussen wants to expand its catalyst market base, contribute to meeting emissions targets and reduce the net consumption of noble and scarce metals in their product range.

Dynea AS is a Norwegian-owned company for wood adhesives production, industrial coatings and licensing of Silver Formaldehyde plants with productions sites in Norway, Denmark and Hungary. Dynea holds several unique technologies for licensing, and its further technology R&D is based in Norway. In iCSI, Dynea aims to continue its technological leadership in formalin production for improved plant operations and reduced cost, as well as increase its licensing.

INOVYN Ltd. is a leading producer of chlorvinyls and associated products, wholly owned by INEOS. INOVYN has 8 European production sites and 4300 employees, of which INOVYN Norway AS constitutes about 300 employees in two sites: The chlorine/VCM production at Rafnes and the PVC plant at Herøya. Through iCSI, INOVYN wants to further improve the VCM technology to achieve world class energy and raw material efficiency.

Haldor Topsøe AS is a catalyst producer and process plant technology developer based in Denmark. Topsøe is known for its emphasis on research and scientific excellence as a basis for its business. In iCSI, Topsøe aims to explore new, direct routes from lower alkanes to bulk chemicals, thereby expanding their technology range and potentially reducing the energy consumption and emissions associated with such production.

Centre Board

The Board is the decision-making body for the execution of iCSI's vision and objectives. Its functions and mandate are described in the iCSI Consortium Agreement: "The Centre Board shall ensure that the intentions and plans underlying the Contract for the Project are fulfilled, and that the activities discussed in the Project description and the Work Plan are completed within the approved time frame. The Centre Board will further ensure that the interaction between the Centre, the Host institution and the other Consortium participants functions smoothly ". Each partner is represented (permanent + deputy) and has one vote. The Research Council of Norway is represented by an observer.

The board members since August 2019 are:

Dr. Pablo Beato

Lead Scientist at Haldor Topsøe, directing the Atomic-Scale Analysis department.

Johan Skjelstad

Project Manager at K A Rasmussen.

Lars Axelsen

General Manager of Technology Sales & Licensing at Dynea.

Dr. Marco Piccinici

Vinyl Chloride Monomer and Organic Chlorine Derivatives Research Manager at INOVYN

Torgeir Lunde

Head of Ammonia/ Nitric Acid Technology at Yara Technology Centre at Yara International

Professor Einar Uggerud

Head of Department of Chemistry at University of Oslo

Professor Karina Mathisen

Vice Dean for Education and Dissemination at the Faculty of Natural Sciences, NTNU

Dr. Duncan Akporiaye

Research Director at SINTEF Industry.

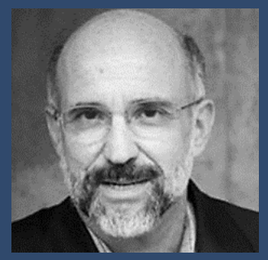
Dr. Aase Marie Hundere

Special advisor RCN, with Responsibility for Nanotechnology and Advanced Materials

Scientific Advisory Committee

Prof. Alessandra Beretta

Politecnico di Milano, Italy



Prof. Enrique Iglesia

University of California, Berkeley, USA

Prof. Graham Hutchings

Cardiff University, United Kingdom

Three renowned scientists from prominent institutions who have excelled within iCSI-relevant areas of heterogeneous catalysis have committed to contribute to iCSI and act as inspiration for the iCSI researchers. Their main tasks are to advise the iCSI Board on the ongoing work in the Centre, to participate and interact with the young researchers at the iCSI Annual Seminar, and to promote iCSI's internationalization and recognition.

Management and Administration

The Centre is hosted by the Department of Chemical Engineering at NTNU. The administration team consists of a Centre Director, a Coordinator/Vice Director and an Economy Adviser. In 2019, the increased administrative responsibilities that followed the Midway Evaluation of the Centre's for Research-based Innovation generation III (SFI-III) led to a temporary extension of the coordinator team to three part-time members from August 2018 to May 2019. All coordinators have experience from academic and/or industrial research.

Hilde Johnsen Venvik

Professor
iCSI Centre Director

Torgrim Mathisen

Senior Executive Officer
iCSI Economy advisor

Anne Hoff

Senior advisor
iCSI Coordinator

Estelle Vanhaecke

Senior advisor
iCSI Coordinator

Nikolaos Tsakoumis

Researcher
iCSI Coordinator

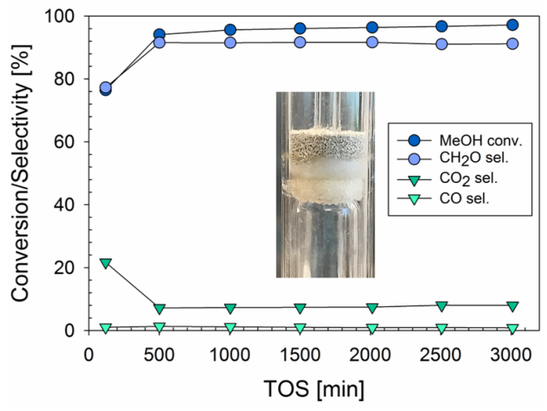
Scientific Highlight 2019

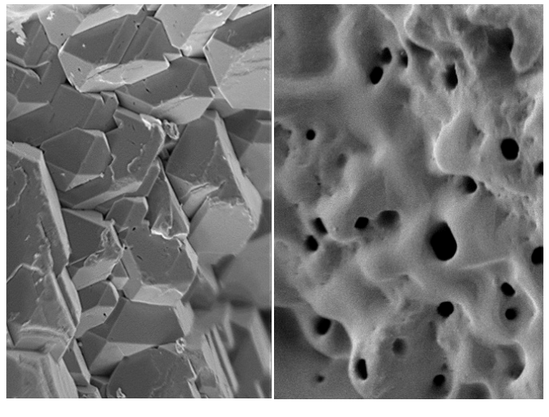
The first iCSI publication from iCSI Industrial Innovation Area 3 (IIA3) came out in 2019! IIA3 is called Frontier formalin technology development, and formalin (formaldehyde in aqueous solution) is a widely used base chemical, for example in adhesives and resins in the wood industry. Under industrial reaction conditions, some of the feedstock (methanol) and/or product (formaldehyde) is lost to CO and CO_2, and the iCSI team of industrial and academic researchers are exploring the possibilities for suppressing this formation. The main target in IIA3 is to improve the selectivity to formaldehyde of the process that uses silver (Ag) as a catalyst for the oxidation of methanol to formaldehyde through a fundamental understanding of the reaction and the silver catalyst surface.

The publication came out in Volume 62 of the journal Topics in Catalysis, containing selected papers from the 18th Nordic Symposium on Catalysis, Copenhagen, 26-28 August 2018. PhD student Stine Lervold received a special invitation to publish after winning the prize for best poster at the conference. The work is a joint effort between the industrial researchers at Dynea and KA Rasmussen, and NTNU and SINTEF. Two NTNU Master students also contributed.

In the study, we compare experiments under industrially relevant conditions with high formaldehyde selectivity (>90%) to model exposures, for example methanol and steam alone. From this it was found that the massive morphological changes of the electrolytic silver catalyst particles under methanol-to-formaldehyde reaction conditions at 650 °C are mainly an effect of oxygen (O_2) in the gas phase (fresh catalyst in left picture, after reaction in right picture). Hence, while the results confirm the role of dissolved O to the restructuring phenomena discussed by many authors, dissolved H appears not to be prerequisite, which contrasts with several claims. The interested reader will find additional details and conclusions on page 34!

Typical product from use of adhesives and resins in the wood industry





Conversion of methanol and product selectivity. Fresh catalyst in left picture, post-reaction in right picture.

Reference: *S. Lervold, K. Arnesen, N. Beck, R. Lødeng, J. Yang, K. Bingen, J. Skjelstad and H.J. Venvik, Morphology and Activity of Electrolytic Silver Catalyst for Partial Oxidation of Methanol to Formaldehyde Under Different Exposures and Oxidation Reactions. Top Catal 62, 699–711 (2019). https://doi.org/10.1007/s11244-019-01159-0*

iCSI Moments 2019

Midway Evaluation

On April 1, 2019, iCSI had a site visit from the international expert panel engaged by the Research Council of Norway (RCN). The panelists included generalists Professor Alison McKay from the University of Leeds and Mattias Lundberg from the Swedish Foundation for Strategic Research (SSF), and scientific experts Associate Professor Ilenia Rossetti from the University of Milan and Professor Lars Pettersson from the KTH Royal Institute of Technology, Sweden. The panel's findings and views of the Centre were reported to RCN, whose Board confirmed on September 9, 2019:

The Centre will be continued for a new three-year period without the implementation of specific measures as a result of the evaluation.

RCN's recommendation to the Board included the following:

...The panel appreciates the Centre's balance between basic research and topics of a more applied nature. Choosing applied issues directly contributes to deeper insight and opportunities for improvement of established industrial processes. The panel concludes that this is an excellent centre that conducts research that is internationally competitive and addresses relevant issues identified by the Centre's industrial partners. Scientific production is high and at a good and sometimes excellent level.... The Centre has engaged internationally profiled professionals in a Scientific Advisory Committee (SAC) that provides constructive input to the Centre and individual feedback to PhD fellows. The fellows at the Centre are motivated and value collaboration and dialogue across work packages. The panel recommends that the Centre continue to facilitate various measures for mobility – both internationally and to / from business.....The Centre's recent initiative towards Process 21 and positioning in relation to the EU are important measures in this direction. The Centre has good management and good support in the host institution and with partners.....All industry partners are active on the Board and have clear objectives for participation in the Centre..... In the past three years, the Centre has been encouraged to allocate more resources to research projects that have industrial interest.

Visit from SAC member Enrique Iglesia

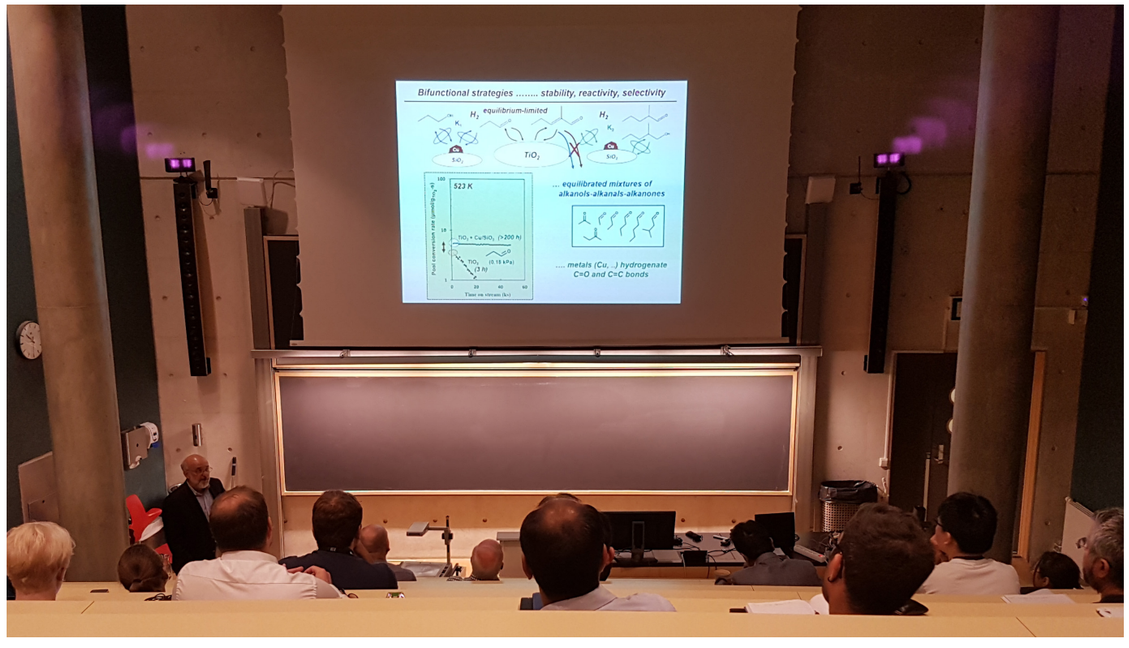
Enrique Iglesia, a member of the iCSI Scientific Advisory Committee, was the recipient of the 2019 Michel Boudart Award for the Advancement of Catalysis. The Michel Boudart Award recognizes and encourages individual contributions to the elucidation of the mechanism and active sites involved in catalytic phenomena and to the development of new methods or concepts that advance the understanding and/or practice of heterogeneous catalysis.

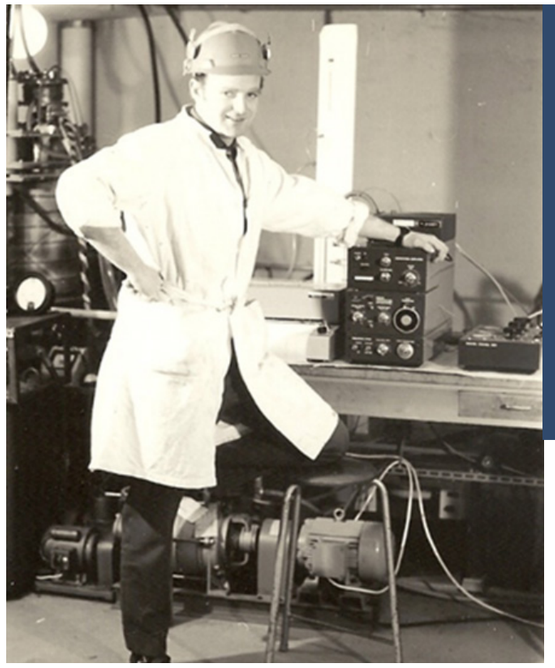
The Award is sponsored by the Haldor Topsøe Company, and is administered jointly by the North American Catalysis Society and the European Federation of Catalysis Societies.

Professor Iglesia and his research group have advanced the design, synthesis, and structural and mechanistic characterization of solid catalysts for chemical reactions involved in the production, conversion, and use of energy carriers, in sustainable syntheses of chemicals and intermediates, and in the protection of the environment.

In August 2019, Professor Enrique Iglesia contributed to iCSI with full-day visits first at NTNU and then at UiO. At both sites he gave an inspiring guest lecture, entitled *C-C Coupling and O-atom Removal in Oxygenate Reactions at Lewis Acid-Base Pairs on Oxide Surfaces.* The rest of the day was spent on individual meetings with PhD candidates and Postdocs (NTNU) and meetings with the various iCSI project teams (UiO). The candidates were grateful to have this opportunity for inspiring discussions and were very impressed both with Professor Iglesia's broad practical experience and his overview of various topics and issues.

iCSI is proud and pleased to have a professional capacity like this in the Scientific Advisory Committee. We admire his endurance through the two days of program from early morning to late evening.





"Norway is a small country. Spending some time in a good laboratory abroad should have high priority."

"Take feedback on manuscripts seriously. The reviewers might have some good points!"

- Anders Holmen

Anders as a SINTEF research scientist in the group led by docent Solbakken in front of the acetylene rig

Researcher Portrait

Professor Emeritus Anders Holmen

When Anders Holmen received the Statoil (now Equinor) Researcher Award in 1994, it was reasoned that 'he has the primary responsibility for building up a recognized international research environment in the field of industrial reaction catalysis at both NTH and SINTEF. He has initiated research on chemical processes of vital interest to Statoil in petrochemicals, refining and gas conversion. Particularly groundbreaking is his work on coking and deactivating of catalysts. Within octane processes, a test and development laboratory has been set up and the laboratory is still operating. He has also initiated the construction of an advanced surface laboratory for atomic level analysis, as well as educated most of the chemical engineers working at Statoil.'

Later, this recognition was confirmed when he received NGCB's Award for Excellence in Natural Gas Conversion in 2010 for 'his achievements in advancing concepts and practical applications of direct and indirect routes for the efficient utilization of natural gas....Throughout his career, Holmen has contributed to the understanding and practice of Fischer-Tropsch synthesis, specifically by unravelling the complex effects of water on reaction rate and selectivity and the role of Co crystallite size and of supports on catalyst reactivity and stability.'

So, how did Anders Holmen accomplish this?
After graduating from Department of Chemical Engineering at NTH in 1966, he started to work for SINTEF Applied Chemistry. This was not (according to him) due to a wish for a research career, but because the job was close to good friends in Trondheim and his family in Østerdalen.

Åge Solbakken was an important mentor for Anders, and he also found inspiration in the lectures of visiting Professor Paul Emmett at NTNU in the late 1960s. But what really mattered on his academic path was the year he spent in the laboratory of Professor Michel Boudart at Stanford University from 1978 to 1979. Upon returning to Norway, a position in the Department of Industrial Chemistry was waiting for him, and in 1984 he was appointed as a professor.

Inspired by Michel Boudart, Anders developed a catalysis group. His first PhD candidate from 1985, Edd Blekkan, is still a close colleague at the department. More PhD candidates followed on a continuous basis, nearly two of them every year. Anders' list of 50 PhDs ended with Andreas Helland Lillebø in 2014. The professor is very pleased to see that so many of his students have prominent positions in industry, and also that 17 of the PhD candidates were women. Some of them are researchers for SINTEF, and 4 of the 5 professors in the NTNU catalysis group have been his students.

In 1969 oil and gas were discovered in the North Sea and the utilization of these feedstocks become an important part of Anders' work for many years. But even before the discovery of oil and gas, activation of methane, in particular the production of acetylene, was an important subject. The work in the catalysis group was founded by the Research Council (NTNF) and Norsk Hydro, and later, also by Statoil. The more fundamental PhD work was also supported by Norwegian Industry, due to a great demand for well-educated people.

"Reaction mechanisms come and go, but the results from proper experimental studies remain unchanged."

One key factor in the success of the catalysis group is a large park of pilot plants – some optimized to simulate industrial processes, others achieving high quality kinetic data. The pilot plants, along with access to a number of advanced, state-of-the-art catalyst characterization methods, such as Auger spectroscopy, Scanning Tunneling Microscopy (STM), Electron Microscopy (SEM/TEM) and X-ray Photoelectron Spectroscopy (XPS) have been crucial for the results. Modern techniques such as TEOM (microbalance) and SSITKA (transient kinetics) were introduced and TAP (temporal analysis of products) were used in co-operation with laboratories outside Norway. The use of X-ray absorption spectroscopy and other synchrotron techniques is also important for the work in the group. The use of TEOM was pioneered by the catalysis group in studying coke formation and diffusion in microporous catalysts.

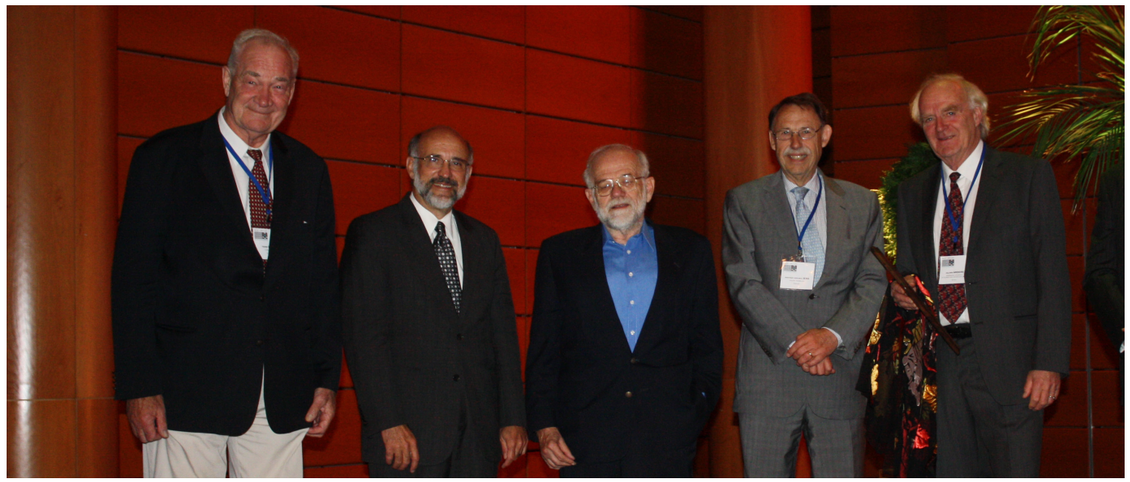
"Be sure that you measure what you want to measure and not something else, such as rates influenced by diffusion."

Development of the laboratories has been possible through the tight collaboration with Norwegian industry over the years. But contributions from the university and participation in long-running programmes supported by the Research Council, such as SPUNG, InGAP and now iCSI, have been invaluable in the long-term development of the group's high professional level.

The professor explains that heterogeneous catalysis takes place on the surfaces of solid materials. Therefore, thorough knowledge of the surface is important. New or improved techniques for surface studies are continuously being developed. In recent years we have also seen tremendous development in theoretical methods for describing surface reactions. Catalysis researchers must have an open mind for all these new methods. However, we will not succeed without hard-working people who have an eye for quality and an understanding of all the traps you can walk into. The catalysis group is doing very well and maintains a high standard of teaching and research, which makes it a pleasure for Anders to follow the work closely. He is also very pleased about the social life in the group and to see that the group follows the tradition of celebrating the PhD candidates. Education of the candidates is of course a very important part of the University work – maybe the most important!

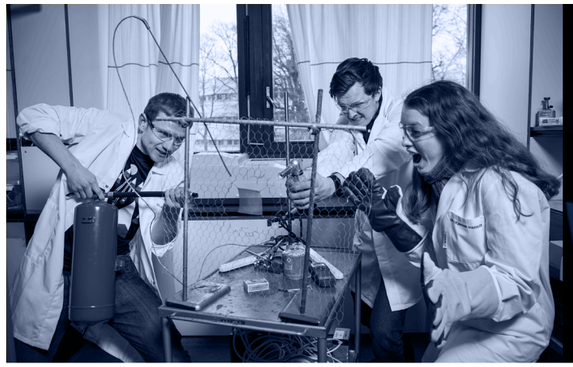
"If you do not apply for a grant or a research project – you can be sure that you won't get anything."

'I feel very privileged to spend my Emeritus time in the Catalysis Group', Anders says. It gives him the possibility to follow the trends in modern catalysis and to write up unpublished work. Together with his wife Bjørg, he also appreciates spending time with his three grandchildren who live close by. 'Life is good for this old man!' he says.



A proud moment 2010: On the podium with former recipients of the NGCB award, from left: David Trimm, Enrique Iglesia, Lanny Schmidt, Jens Rostrup-Nielsen and Anders Holmen

iCSI Moments 2019



Fun at the lab

Celebration - Midway evaluation passed!

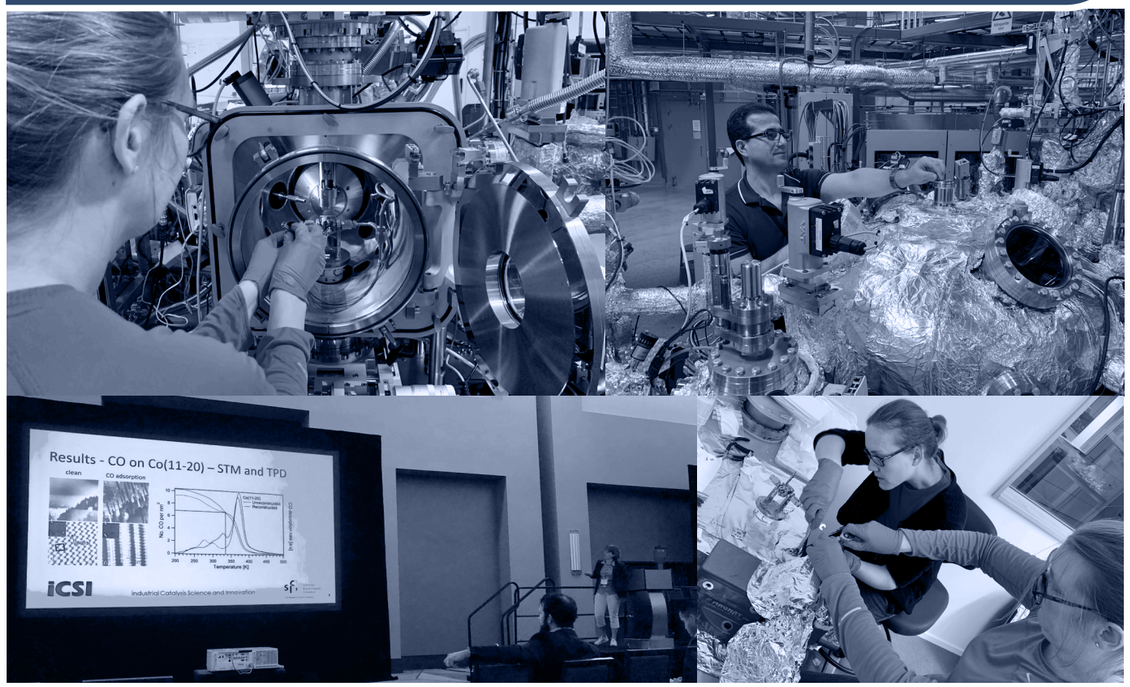
Diligent master students

New PhDs

Ladies night at NTNU

Industry and research partners' meetings

Beam time @MAXIV



Researchers' Corner

Two new PhD candidates, Karoline Kvande and Julie Hessevik, joined iCSI in 2019

"When it comes to be a part of an SFI, I think it's especially nice that we have such a close collaboration with the industry. This gives me a closer insight into how things work outside the university and we become more focused on how to develop ourselves and the process further. I also hope that it will count positively in my further career."

- PhD candidate Karoline Kvande

Karoline started in April 2019 in the Catalysis Section at UiO with Stian Svelle as her main supervisor. The overall objective of her PhD project is to measure the activity of transition metal containing porous catalysts in the continuous catalytic process for the direct activation of lower alkanes.

Karoline likes being busy. She took both her Bachelor's and Master's degrees in chemistry at the University of Oslo and at the same time, she worked as a kayak trainer and was very active in Realistforeningen at the university. Now, she says, 'the best thing about being a PhD student is all the opportunities I have to experience and learn new things! I learn something new every day at work, and I really enjoy the challenges of everyday life. Of course, it can be frustrating at times, but it only adds to the joy when problems are solved. In addition, I think it is so nice that there are many different offerings in the form of events, courses and conferences that I can attend. I try as best I can to throw myself into it, to get as much as possible out of these 4 years.' However, trying to meet a variety of deadlines simultaneously, when she would rather be doing experiments and other things, makes Karoline's life a little busy. Sometimes she just wishes she had a few more hours in the day.

Her dream career is at a place where she can continue with research and development. Right now, she considers entering industry as her best option, but it certainly depends on what kind of opportunities exist when she finishes her studies. Maybe there will be an exciting postdoc, or maybe something completely different will tempt her. She feels pretty open to new opportunities.

About life outside the university, she says, 'I'm generally happy to learn new things and often have many small projects going on, also outside of job. But my regular activities in everyday life are experimenting in the kitchen with new and exciting foods, as well as keeping myself active through paddling, strength training and good walks. Otherwise, I love being social, so I try to find time for friends and family as often as I can.' We wish Karoline all the best for her research and the other parts of her life.

Julie joined the NAFUMA group in December. Together with Helmer Fjellvåg and Anja Olafsen Sjåstad as supervisors, she will study catchment of platinum group metals. The objective is to investigate how such metals are transported in the gas phase under process conditions and how these can be recovered/captured by metals and by metal oxide catchment gauzes.

Julie had experience from a variety of areas and institutions before she joined iCSI. She obtained her Bachelor's degree in nanotechnology and her Master's degree in nanoscience from the University of Bergen. For her Master's thesis she worked on the synthesis, characterization and testing of catalysts (homogeneous and heterogeneous) for copolymerization of CO_2 and epoxides. At university, she also found time to serve as a board member of the student council for Nanotechnology/Nanoscience students at the University of Bergen. Following her studies, she worked as an engineer in NTNU's Department of Materials Science and Engineering for one year and later in the start-up company CrayoNano for two years.

Now, back at university, she appreciates the opportunity to dig into details on interesting topics. As a relatively recent PhD candidate, Julie's biggest challenges so far have been coordinating the various activities at the start of a PhD – teaching, taking classes, seminars and working on her project.

Like Karoline, Julie is also very happy to be part of a centre for research-based innovation (SFI). 'It's nice to see that industry is interested in the research, and that's an additional motivating factor for me. We often have meetings with our industry partners, which gives us the chance to work on and discuss complex issues with more people, who have other kinds of experience', she says.

For the future, she doesn't want to limit herself to a specific career path yet. 'I like challenges and enjoy research, technology development and project work. What I envision that would be fun is being able to do project-based work in a company or research institution, but I'm open to various opportunities that may arise along the way'.

And when not at work: Julie loves to be physically active, especially through climbing and other outdoor activities.

"The best part of life as a PhD candidate is that you have the opportunity to go into depth on a topic you are interested in, as well as the flexibility you have."

- PhD candidate Julie Hessevik

Exchange Programme 2019

Stine Lervold

- PhD candidate

iCSI's industry partners are actively involved in the research programmes and offer a two-month industry exchange programme to the PhD candidates. This is a unique opportunity for the candidates to gain experience with industrial challenges and thinking. In 2019, the three candidates Stine Lervold, Samuel Regli and Endre Fenes from iCSI took advantage of this opportunity and visited Dynea and KA Rasmussen, Haldor Topsøe and Inovyn, respectively.

Stine is a PhD candidate focusing on improving the performance of the existing formalin production process technology (WP 3.1). During 2018/2019 she completed a two-month internship at Dynea AS and KA Rasmussen AS through the iCSI industrial exchange programme.

"I did my exchange at both of my industrial partners, KA Rasmussen and Dynea. During this period, I got to experience the industrial aspect of formaldehyde production, but also the origin of the silver catalyst. Having the opportunity to experience the process first-hand broadened my perspective beyond the lab and gave me a better understanding of the importance of my PhD work. While experiencing parts of the industry relevant for the MTF process, I was also challenged with other tasks industry encounters.

This has been a unique chance to meet others, and interact and exchange ideas in a new and inspiring environment. Not only has this benefited my development as a scientist, but it also gave me a glimpse of what the future could look like after finishing my degree. I highly encourage other iCSI researchers to use this opportunity to get to know our industrial partners."

Not only PhD candidates benefit from the exchange. Stine's host at KA Rasmussen and iCSI board member, Johan Skjelstad, has this comment on the value created for KA Rasmussen:

'The PhD student exchange yielded a great benefit in the form of a study on new production methods. This would not have been possible without NTNU's research training and methodology in attacking new problems'.

Scientific Activities

iCSI main Industrial Innovation Areas (IIAs) and Work Packages (WP):

IIA1

21st Century Ammonia Oxidation and Nitric Acid technology development

WP1.1 WP1.2 WP1.3

NTNU · UiO : University of Oslo · SINTEF · YARA · K.A.Rasmussen Norway

IIA2

New NOxabatement technologies for the marine market and state-of-the-art SCR catalysis

WP2.1

SINTEF · YARA

IIA3

Frontier formalin technology development

WP3.1 WP3.2 WP3.3

NTNU · SINTEF · K.A.Rasmussen Norway · dynea

IIA4

PVC Value Chain: World class energy and raw material efficiency for the production of Chlorine and Vinyl Chloride Monomer (VCM)

WP4.1 WP4.2 WP4.3 WP4.1

NTNU · SINTEF · inovyn

IIA5

The next step in direct activation of lower alkanes

WP5.1 WP5.2 WP5.3

HALDOR TOPSOE · SINTEF · UiO : University of Oslo

IIA6

Generic projects for additional industrial synergies

WP6.1 WP6.2 WP6.3 WP6.4

NTNU · UiO : University of Oslo · SINTEF · dynea · inovyn · HALDOR TOPSOE · YARA

Scientific Activities

IIA1: 21st Century Ammonia Oxidation and Nitric Acid Technology Development

The Team in 2019

Anja Olafsen Sjåstad	UiO	IIA leader, PhD supervisor and WP responsible (WP1.1), advisor (WP1.2)
David Waller	YARA	Industrial senior (Yara), PhD supervisor (WP1.1), industry researcher (WP1.2-1.3)
Helmer Fjellvåg	UiO	Advisor (WP1.1-1.2)
Asbjørn Slagtern Fjellvåg	UiO	PhD candidate (WP1.1)
Julie Hessevik	UiO	PhD candidate (WP1.1)
Susmit Kumar	UiO	Researcher (WP1.1)
Oskar Iveland	UiO	Master student (WP1.1)
Oleksii Ivashenko	UiO	Postdoctoral fellow (WP 1.1)
Sang Baek Shin	YARA	Industry researcher (WP 1.3)
Ketil Evjedal	YARA	Industry researcher (WP 1.1)
Malin Bjørneboe	YARA	Industry researcher (WP 1.1)
Van Giau Nguyen	YARA	Industry researcher (WP 1.1)
Ant Clasen	YARA	Industry researcher (WP 1.1)
Torgeir Lunde	YARA	Industry researcher (WP 1.1-1.2)
Johan Skjelstad	KA Rasmussen	Industry Researcher (WP1.1-1.2)
Thomas By	KA Rasmussen	Industry Researcher (WP1.1-1.2)
Silje Fosse Håkonsen	SINTEF	Researcher WP responsible (WP1.2)
Børge Holme	SINTEF	Researcher (WP1.2)
Magnus Rønning	NTNU	PhD supervisor, WP responsible (WP1.3)
Rune Lødeng	SINTEF	PhD supervisor, researcher (WP1.3)
Ata Al Rauf Salman	NTNU	PhD candidate (WP1.3)
Minadir Saracevic	NTNU	Master student (WP1.3)
Bjørn Christian Enger	SINTEF	Researcher (WP1.3)

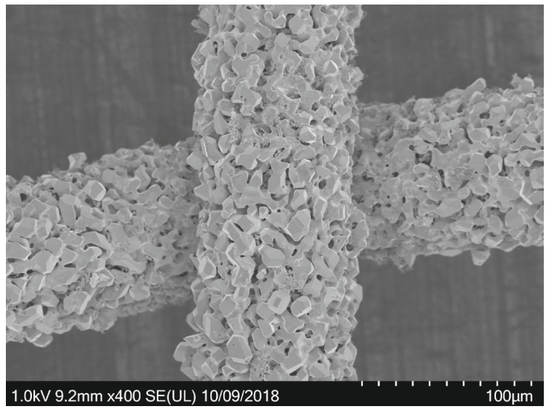
Motivation
Nitric acid is a valuable commodity chemical with an annual global production of about 65 million tonnes. The production is a three-step process where NH_3 is first oxidized to NO over a Pt-Rh gauze catalyst at high temperature, and this is followed by a homogeneous gas phase oxidation of NO to NO_2 at moderate temperatures. Finally, the nitric acid is obtained by absorption of NO_2 in water. A major technological challenge is loss of Pt and Rh in the highly exothermic first step. To avoid permanent loss and costly noble metal recovery, an optimized catchment (recovery) system is required.

This is targeted in WP1.1 and WP1.2 through investigating fundamental aspects of PGM species volatilization and transport, as well as surface reaction and reconstruction, gas absorption and diffusion into the solid phase catchment system. WP1.3 concerns the development of new catalyst technology for oxidation of NO to NO_2, which would reduce future capital investments and increase the energy recovery if the bulky homogeneous oxidation system could be replaced by a compact, heterogeneously catalyzed process.

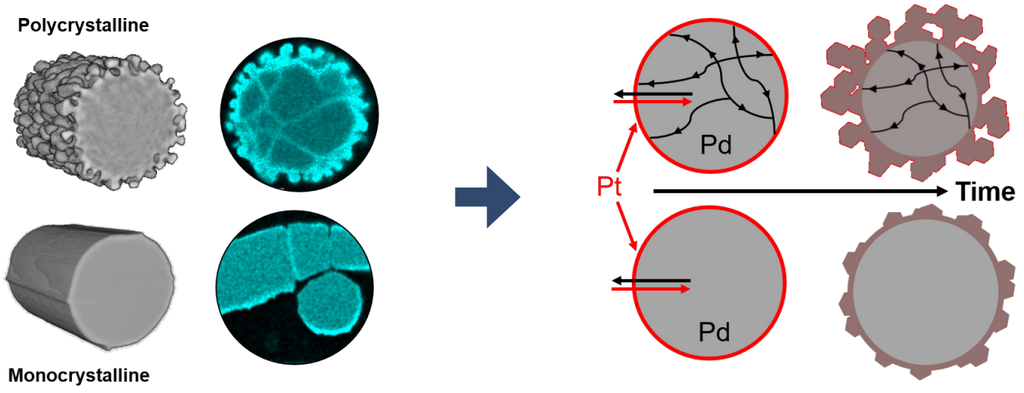
Publication
Publications and conference contributions from IIA1 are listed in page 58

Reconstruction of Pd-Ni catchment gauzes during high temperature ammonia oxidation

The financial cost of Pt-loss during ammonia oxidation is one of the largest single expenses in nitric acid production. The current commercial Pd/Ni catchment unit can capture the lost Pt with high efficiency with simple handling in the reactor. Unfortunately, the Pd/Ni alloy is victim to severe grain reconstruction during the Pt-catchment process (picture at top) This causes problems with pressure drop in the ammonia oxidation reactor, and it can therefore not be used to its full potential. Via in-situ tomography experiments at ESRF we have mapped the development of the morphology of pure Pd and Pd/Ni wires during this Pt-catchment process. Combined with home lab experiments, we have seen the impact of the grain boundary structure on the grain reconstruction phenomena, and how different diffusion rates come into play. When Pt is captured on the surface of the Pd (or Pd/Ni) wire, a flux of rapidly diffusing Pd atoms move in the grain boundaries and towards the surface, meeting the Pt incoming from the gas phase. In the end, this causes the grain boundaries to crack open and grain reconstruction to occur (figure at right). This strongly resembles corrosion on base metal alloys and their oxidation behaviour. In other words, we do not see corrosion by oxidation, but by platination.



Pd/Ni gauze after 20 days in the pilot plant.



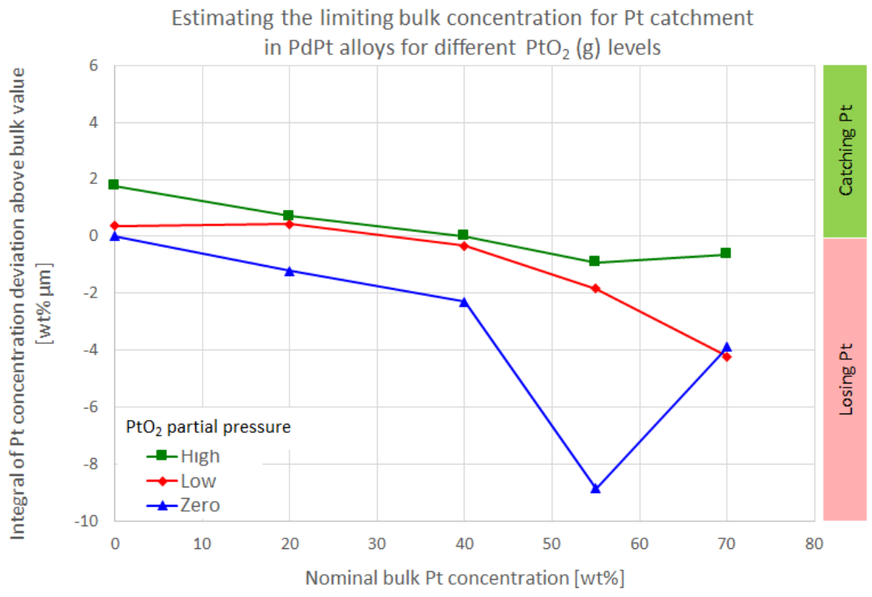
Visual schematic of the development of pure Pd-gauzes during Pt-catchment. To the left, experimental results showing the difference between poly- and mono-crystalline wires. Especially visible are the diffusion in grain boundaries in the polycrystalline wire, and the diffusion limitation in the monocrystalline wire. At right is how we interpret this in our model for corrosion by platination.

Experimental investigations of Pt/PtRh volatilization and catchment

A dedicated six-zone reactor system is used to generate PtO_2 vapor in dry air/inert gas mixture and subsequent catchment on pure Pd and Pd-Pt binary alloys. The furnace is optimized to provide temperature gradients in the range 800-1200°C, representative of those used between the location for the Pt volatilization in the ammonia oxidation step and the catchment material in the industrial process.

A set of polished Pd and Pd-Pt discs with diameters of 5-6 mm and different Pd-Pt compositions have been exposed to a flow of PtO_2 vapor for four hours at 900°C. The diffusion profile has subsequently been analysed using Sputtered Neutral particle Mass Spectrometry (SNMS).

Our results show that for the low Pt-containing samples, Pt is picked up from the gas stream and a clear diffusion profile is observed. However, for samples that initially contained high amounts of Pt we measure the opposite effect where Pt is actually lost from the catchment sample under these conditions. This behaviour is more pronounced in the catchment samples containing the most Pt. An interesting observation is that with higher PtO_2 partial pressure, more Pt is caught by the discs (figure below). The turning point (with net zero uptake of Pt) also seems to shift to higher Pt containing alloys when increasing the PtO_2 partial pressure in the gas phase. An unexpected large Pt loss is observed from the Pd45Pt55 sample exposed under zero PtO_2 partial pressure. This point (and others) will be run again to check if this diffusion profile is really valid, and to assess the reproducibility in the data.



Net Pt uptake in Pd and Pd-Pt binary alloys after 4 hours exposure to different PtO_2 partial pressures.

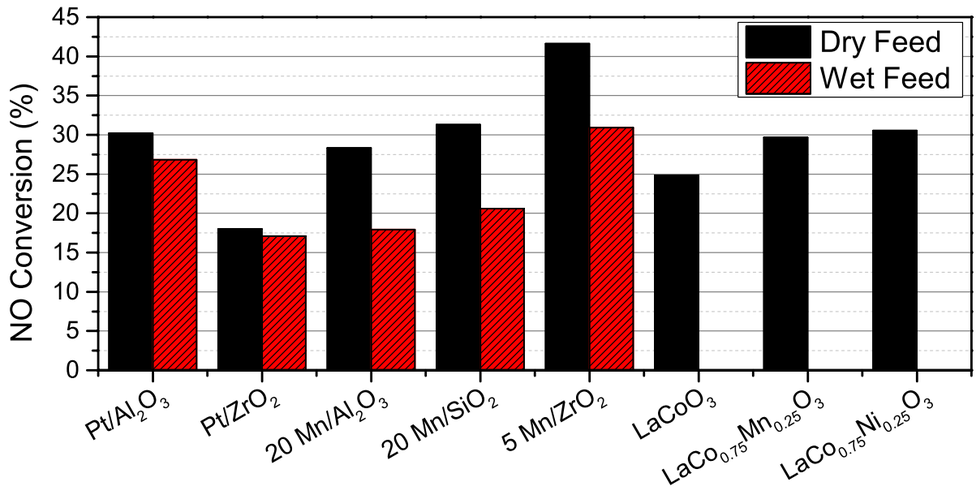
Catalytic oxidation of NO to NO2 for nitric acid production

Replacing the homogenous gas phase oxidation of NO to NO_2 step in nitric acid production with a more compact heterogeneous catalytic process offers several advantages: a) a significant increase in recovery of high-quality heat, b) acceleration of the oxidation reaction and c) potential for a substantial decrease in capital expenditure (CAPEX) for new plants. Some efforts have been made to find a catalyst that is effective under industrial conditions, but to this date, the process is still carried out as a homogeneous reaction in modern nitric acid plants.

The current work aims to find efficient catalysts for oxidation of NO to NO_2, under conditions relevant to nitric acid plants, enabling significant process intensification. This also involves gaining a fundamental understanding of reaction kinetics and the mechanism of oxidation of NO over promising catalysts. The industrial process dictates the conditions of catalytic investigations: feed composition of 10% NO, 6% O_2, 15% H_2O, pressure 1–10 bar and temperatures in the range 150–450 °C.

Mimicking industrial conditions in a laboratory is challenging. A dedicated setup was built that was capable of investigating the activity of powdered catalysts using realistic feed concentrations at atmospheric pressure partially simulating nitric acid plant conditions. The activity of the catalysts was studied as a function of temperature to provide information about the onset temperature of catalytic conversion. The stability of the catalysts was probed by studying catalytic activity as a function of time. Although water is an integral part of the reaction mixture in the nitric acid plant, catalytic experiments were performed in the absence and presence of water to elucidate the effect of water on catalyst activity and structure. The NO conversion levels at 350°C for the various catalysts are presented in the figure below.

Platinum catalysts supported on Al_2O_3 and ZrO_2 are active for the oxidation of NO. But we also seek to identify potential replacements of platinum group metal (PGM) catalysts, exhibiting superior or comparable catalytic activity. Transition metal oxide (manganese) on different support materials (Al_2O_3, SiO_2, ZrO_2) and perovskites ($LaCo_{1-x}B_xO_3$, B = Mn, Ni) were investigated in this respect. The experiments revealed that zirconia-supported catalysts with low manganese loading are promising cost-efficient catalysts for the conversion of NO in nitric acid production.



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

IIA2: Abatement of Nitrogen-containing Pollutants. State-of-the-art SCR Catalysis

The Team in 2019

Jasmina Hafizovic Cavka	SINTEF	IIA leader
David Waller	YARA	Industrial senior Yara, industry researcher (WP2.1)
Silje Fosse Håkonsen	SINTEF	Researcher and WP responsible (WP2.1)
Karl Isak Skau	YARA	Industry researcher (WP2.1)
Martin F. Sunding	SINTEF	Researcher (WP2.1)

Motivation

Selective Catalytic Reduction (SCR) is a core technology in the treatment of exhaust gases (NO_x) from various sources, and the applications are emerging due to stricter emission regulations and circular economy. The most common SCR catalyst technology for power and marine applications is based on vanadium oxides combined with other oxides; typically supported on monolithic structures to allow high throughput and minimum pressure drop for the reduction of NO_x with ammonia (NH_3). Catalyst lifetimes may be as long as 5 years but vary due to differences in their exposure to poisons, dust and soot. It is therefore desirable to rejuvenate or regenerate the SCR catalysts. The former typically involves dust removal and washing to remove surface particulates and soluble deposits but implies difficulties with respect to obtaining full recovery of the activity. Regeneration, on the other hand, may involve the addition of an active phase to recover the original activity. Recovering the catalyst activity in a simpler way would be highly beneficial. This objective is targeted in WP2.1 through first gaining a deeper understanding of the mechanisms causing the catalyst deactivation through thorough characterization of the catalyst at different stages of its lifetime, and then translating this knowledge into new measures.

Commercial catalysts are mainly based on vanadium oxide (V_2O_5) supported on an anatase (TiO_2) carrier. The total load of V_2O_5 is around 1–5 wt% depending on the specific application. To improve chemical and physical properties of the catalyst WO_3 and MoO_3 are also added. The SCR catalysts lifetime is dependent on the application, and the catalyst normally deactivates due to fouling, sintering, poisoning, or a combination of these.

Research project

Commercial vanadia-based SCR monoliths were installed on ships running on low sulphur (S) fuels. Experience from the industry indicates that lowering the S-content in the fuel can cause unexpected problems for the SCR catalyst, such as higher Si deposits on the catalyst.

To understand the cause of deactivation, the characterization toolbox developed in the project was applied to both the fresh catalyst and one catalyst that has been aboard a ship running on mostly ultra-low sulphur fuel. Powder XRD of fresh and spent catalyst did not show significant changes; the support TiO_2 phased remained in its anatase form after exposure to flue gases. Other compounds were detected by the XRD. The BET analysis confirmed a decrease of the available surface area by 22%.

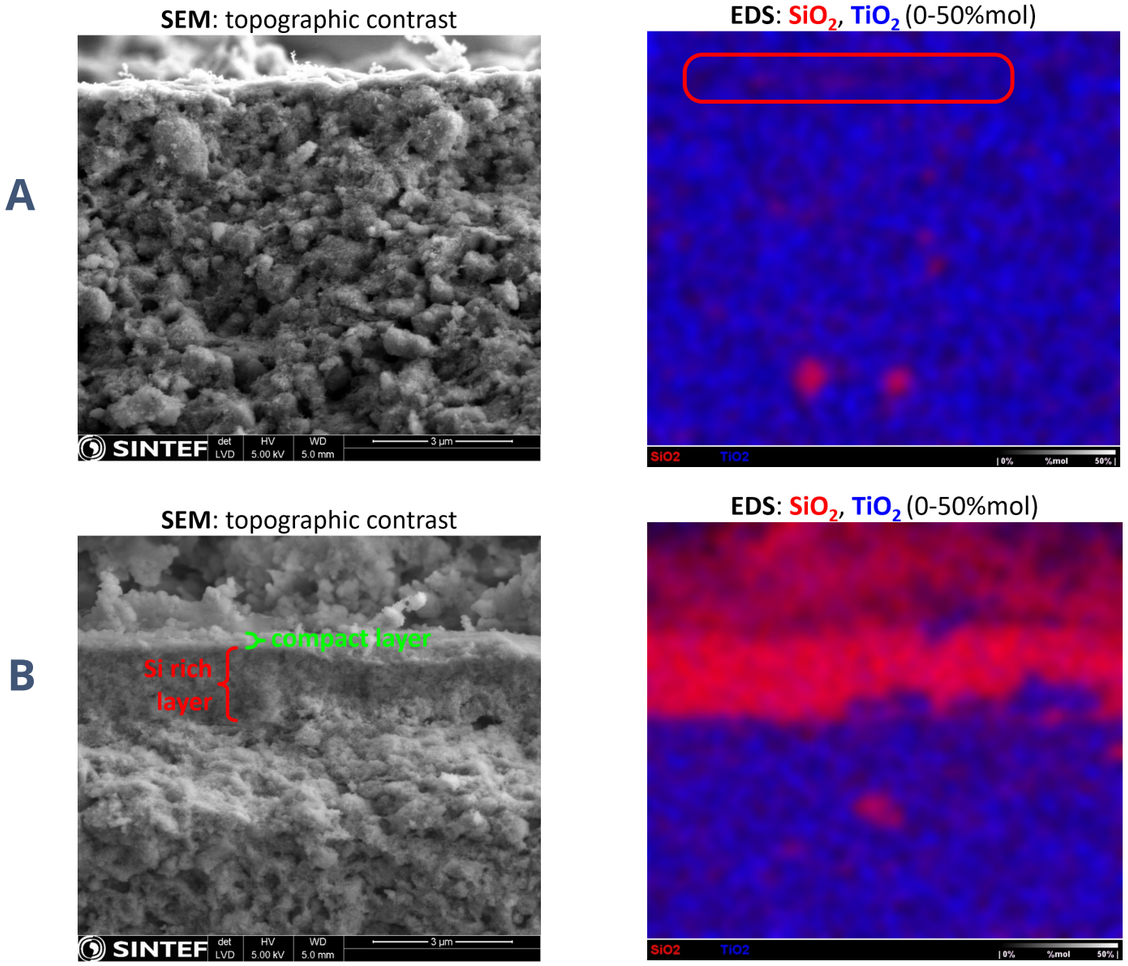
Cross sections of both the fresh and used catalyst were studied by SEM-EDS to look for Si distributions. It was known from before that Si is present in the fresh catalyst in the form of glass fibres used to increase the mechanical strength of the monolith structure. This Si is associated with some other elements. A SEM image and EDS map of the Si layer on the fresh catalyst is shown in part A of the figure below. In addition to these fibres, our results show the presence of a uniform Si-rich layer on both the fresh and used catalysts. In both catalysts a dense film of Si rich (50-100 nm) was observed on the outer surface of the catalyst wall. On the used catalyst a thicker (about 1µm), more porous layer was also detected underneath the dense surface Si rich layer (part B of the figure below).

The source of the thicker Si-rich layer in the used catalyst is not yet clear, but it is believed to originate from the exhaust stream. The Si could potentially diffuse from the fibres to the surface and thereby create Si-rich layers. However, this is not believed to be the primary source of Si, as thicker Si-rich layers have not been observed in used catalysts from other applications. The nature of the Si was further studied by ToF-SIMS to try to shed some light on the origin of the Si. Results revealed the presence of SiO_x near the surface in both the fresh and used samples. No Si-$(CH_3)_x$ groups, commonly found in e.g. silicon oil, were detected.

A diluted HF wash has been utilized to see if it is possible to wash off the Si from the outer surface of the catalyst. Results show that Si is successfully removed, but the wash also has a negative effect on the catalyst itself. However, it may be possible to tune the HF concentration and wash time so as to remove the Si without affecting the catalyst.

Cruise ship in Geirangerfjorden

Photo: Staale Wattø, Sunnmørsposten



A: SEM image and Si EDS map of the fresh catalyst.
B: SEM image and Si EDS map of the catalyst used as SCR catalyst on a ship running mainly on ultra-low sulphur fuel.

IIA3: Frontier Formalin Technology Development

The Team in 2019

Jasmina Hafizovic Cavka	SINTEF	IIA leader
Kristin Bingen	DYNEA	Industrial senior, industry researcher (WP3.1-3.2-3.3), WP responsible (3.2)
Mads Lid	DYNEA	Industry researcher (WP3.2-3.3)
Johan Skjelstad	KA Rasmussen	Industrial senior, industry researcher (WP 3.1)
Thomas By	KA Rasmussen	Industry researcher (WP3.1)
Hilde Venvik	NTNU	PhD supervisor, WP responsible (WP3.1), advisor (WP3.3)
Stine Lervold	NTNU	PhD student (WP3.1)
Rune Lødeng	SINTEF	PhD supervisor (WP3.1), researcher (WP3.2-3.3)
Roman Tschentscher	SINTEF	Researcher (WP3.2-3.3)

Motivation
Formalin is a base chemical that is widely used in adhesives and resins applied in the wood industry. The production proceeds by catalytic oxidation of methanol to formaldehyde, in excess air over a mixed metal oxide catalyst or excess methanol over a silver-based catalyst. Dynea owns both process technologies, and KA Rasmussen is a manufacturer of silver catalysts. The silver process is assumed to have the highest economic improvement potential, due to lower energy consumption and the possibility of increasing the formaldehyde yield beyond 90-92%.

The main objective of IIA3 is improving the formaldehyde yield of the silver-based process. The fast and exothermic nature of the reactions involved requires control of the heat and mass transfer phenomena as well as the surface chemistry proceeding on the silver surface.

Gas phase chemistry may play an additional role at typical reaction temperatures exceeding 600 °C, at which temperature structural changes in the Ag catalyst also occur that are known to affect both the reaction chemistry and the catalyst stability. The lifetime of the catalyst in industrial operation is in the order of months, depending on parameters such as particle morphology, size distribution and the structure of the catalyst bed in addition to the reaction conditions. Further developments are achievable by a more detailed understanding of the reaction conditions and tuning of the silver particle/bed morphology, thus controlling both selectivity and stability.

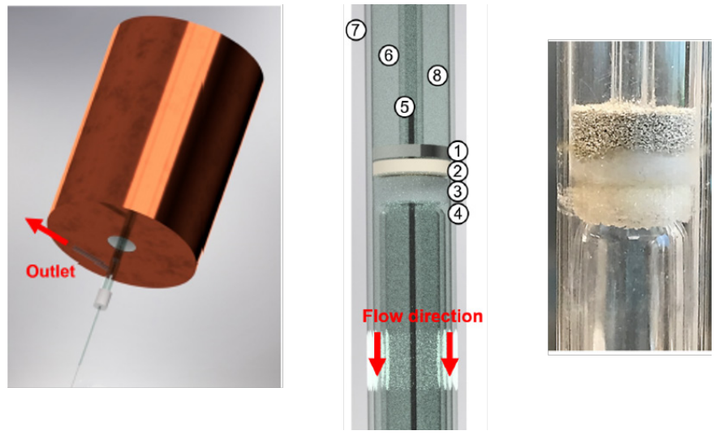
The three work packages are partly integrated through addressing the reaction kinetics and the nature of the Ag species (oxide) affecting the reaction chemistry (WP3.1), the effect of reaction parameters under industrial operation (WP3.2), and further development of mechanistic and reactor models (WP3.3).

Publication
Publications and conference contributions from IIA3 are listed on page 59.

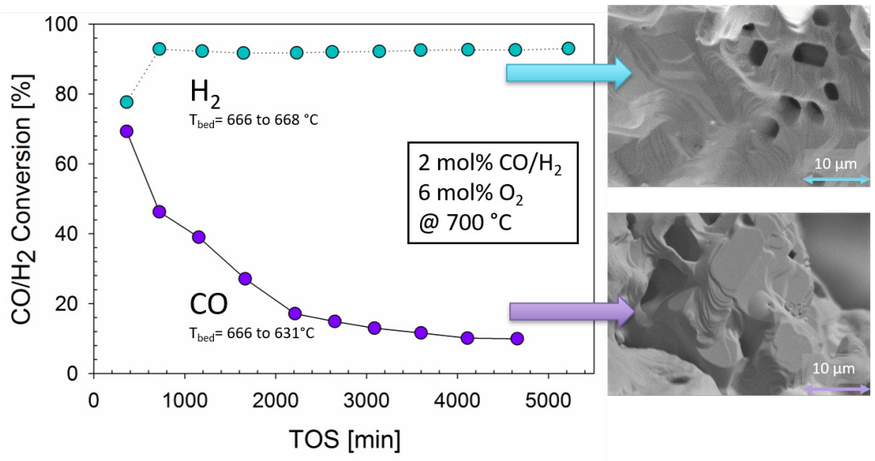
Research 2019
Knowing the relationship between different atmospheres and silver morphology, in conjunction with catalytic activity for oxidation reactions, is important to fully understand the methanol to formaldehyde (MTF) reaction system. In 2019, we reported a study on the interrelationship between morphology changes and the activity of the Ag catalyst. The reactor applied for laboratory methanol, CO and H_2 oxidation experiments is illustrated in the figure at top next page. Specific design measures were implemented in order to mitigate the major challenges involved in studying the MTF reaction at high temperature with good precision. Back-mixing and ignition of the gas phase before the catalyst are suppressed by maintaining a high linear gas velocity and low pressure drop, as well as dividing the heating into two independent zones: preheat at intermediate temperature and reaction at high temperature. Gas phase reactions in the product mixture are suppressed by minimizing void volume and residence time at high temperature. Finally, heat tracing of tubes leading to the analysis is important to avoid polymerization of the formaldehyde product.

The oxidation of H_2 and CO represents reaction subsystems important for optimizing the formaldehyde production process and can provide information on relevant reaction pathways associated with restructuring. Catalysts exposed to oxygen alone, or CO or H_2 oxidation, at temperatures in the range 600- 670 °C undergo severe restructuring of the surface on the mesoscopic scale. A smoothened surface with refaceted areas and pinholes is visible, similar to what is observed after methanol oxidation, industrially as well as in the laboratory experiments (see Highlight on page 12).

The Ag catalyst displays similar, high initial activity for both CO and H_2 oxidation (bottom figure below). However, while the H_2 conversion seems to be facilitated by the restructuring during time on stream, the opposite occurs for CO conversion. This suggests that the CO to CO_2 route is inhibited by the dynamics occurring between Ag and oxygen at high temperature, and that restructured Ag and dissolved O does not promote the CO to CO_2 route at high temperature. Reaction mechanisms that explain CO_2 formation mainly by CO oxidation may need to be reconsidered.



Reactor and furnace design for MTF reaction experiments. a) Illustration of the two-zone heating concept with preheat (15 cm) and reaction zone temperature control (3 cm) b) Sketch of the quartz reactor with (1) catalyst bed, (2) quartz wool, (3) quartz sinter, (4) decreased void volume after catalyst bed, (5) thermocouple, (6) thermocouple pocket, (7) reactor wall, (8) initial void volume before catalyst bed. c) Pre-experiment photo of an Ag catalyst bed inside the quartz reactor with thermocouple pocket on the inside.



Activity and post-reaction surface morphologies of the Ag methanol oxidation to formaldehyde catalyst for CO and H_2 oxidation reaction subsystems.

IIA4: PVC Value Chain: World Class Energy and Raw Material Efficiency for the Production of Chlorine and Vinyl Chloride Monomer (VCM)

The Team in 2019

De Chen	NTNU	IIA leader, PhD supervisor, WP responsible (WP4.1-4.2-4.3)
Terje Fuglerud	INOVYN	Industrial senior, industry researcher (WP4.1-4.2-4.3), PhD supervisor (WP4.1)
Marco Piccinini	INOVYN	Industrial researcher
Endre Fenes	NTNU	PhD student (WP4.1)
Hongfei Ma	NTNU	PhD student (WP4.3)
Yalan Wang	NTNU	Postdoctoral fellow (WP4.1)
Yanying Qi	NTNU	Postdoctoral fellow (WP)
Tho Ba Tran	NTNU	Master student (WP4.1)
Jithin Gopakumar	NTNU	Master student (WP4.1 and WP4.3)
Kumar R. Rout	SINTEF	Researcher (WP4.2), advisor (WP4.1-4.3)
Torbjørn Gjervan	SINTEF	Researcher (WP4.2)

Motivation

Polyvinylchloride (PVC) produced by polymerization of the monomer vinyl chloride (VCM), is the third-most widely produced plastic and finds application in flooring, piping, profiles, cables, etc. VCM production based on ethylene was introduced in the 1950s and is a mature process where high plant reliability and continuous improvement of energy and raw material efficiency is still required to remain competitive and to meet environmental regulations. VCM is produced from ethylene and chlorine in a process involving several chemical conversion steps, one being the oxychlorination of ethylene to EDC, i.e. 1,2 dichloroethane, in a fixed or fluidized bed reactor.

The $CuCl_2/\gamma\text{-}Al_2O_3$ system is the commonly used catalyst in this process, and it is generally agreed that the oxychlorination reaction involves a redox process in which copper cycles between Cu(I)- and Cu(II) states. The oxidation state of the Cu and vacancy concentration of the catalysts play a very important role in determining catalyst activity, selectivity, and stability. It remains a challenge to monitor these properties in situ and provide a principle to tune the vacancy concentration.

Another main challenge of this process is that the Cu(I) forms on the surface of the catalyst during the reaction, thereby causing the aggregation and loss of active Cu. Compounds of alkali and/or rare earth metals are often used as promoters to increase the activity, selectivity and stability. In the project, the promoter effects on reduction, oxidation, and steady-state reactions are studied experimentally and theoretically. The aim is to provide more detailed scientific insights to active sites, the effect of such promoters, and eventually to identify descriptors for the promoter effects that enable rational catalyst design principles.

An operando fixed bed reactor set-up combined with UV/Vis- and mass spectroscopy has been established at NTNU to measure spatial-time quantitative kinetics of the reaction while characterizing the active catalyst component involved. A strategy of combined transient- and steady-state kinetic investigations then enables prediction of the reaction rate and the copper oxidation state at steady-state conditions.

Publication

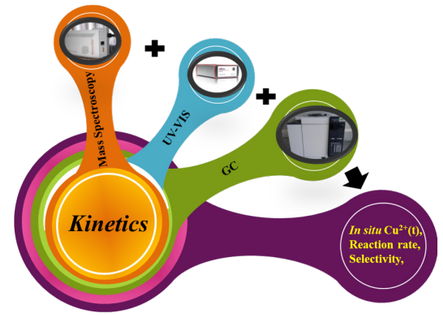
Publications and conference contributions from IIA4 are listed on page 59.

Ethylene Oxychlorination to 1,2 Dichloroethane (EDC), Kinetic Investigations, Modelling and In-situ Characterization

The catalytic cycle of ethylene oxychlorination has been studied by a combined experimental and theoretical approach. The activity and selectivity, as well as the evolution of active sites during the reduction, oxidation and hydrochlorination steps, as well as at steady-state conditions, was studied experimentally by the combined UN-VIS-NIR and MS spectra. The DFT calculation was carried out to obtain a structural atomistic motif of the active site, and the catalytic elementary steps in the catalytic cycle.

The kinetic model developed was also based on the $CuCl_2/Al_2O_3$ and K-doped $CuCl_2/Al_2O_3$ catalysts. The proposed model fits well with the experimental results and can be used to describe the reaction rate and Cu^{2+} (the active Cu species) concentration during the steady state.

It was reported that the $CuCl_2$ is dispersed as a monolayer on the Al_2O_3 surface. Therefore, the influence on Cu caused by support facet can be significant on ethylene oxychlorination. We prepared two types of supports with different morphologies – one platelet, one tubular, and specific facets exposed. They are used as the supports of $CuCl_2$ and evaluated in ethylene oxychlorination. It was demonstrated that the $5Cu/Al_2O_3$-P, with platelet structure and (110) termination, had a higher ethylene conversion and stability than that of $5Cu/Al_2O_3$-T, with tubular structure and (111) termination. Kinetic analysis



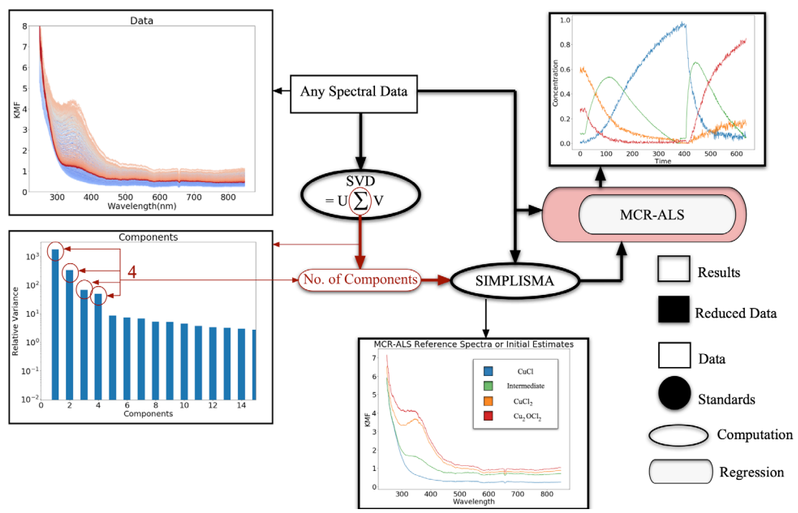
proved that the oxidation rate can be greatly enhanced by the $5Cu/Al_2O_3$-P, and this is important also for the regeneration of the active Cu^{2+}.

Promoter effects on ethylene oxychlorination

$CuCl_2/Al_2O_3$-based catalyst is commonly used as a commercial catalyst in the industry, while dopants like alkali metals are used as the promoters. The main objective of the project is to gain a better understanding of the promoter effect on ethylene oxychlorination from the view of kinetics.

A multiwavelength analysis method using chemometrics has been developed in the project to analyse the UV-VIS-NIR spectra. Multivariate Curve Resolution with Alternating Least Squares (MCR-ALS) was used to analyse and interpret these spectra. A program algorithm for deep data analysis (DDA has been established, where the key compounds and their standard spectra, as well as the changes of these components over time, are obtained.

The effects of promoters such as metal (K, Li, Na, Rb, Ce, La, Mg, Ca, etc) chlorides on the catalytic performance at steady-state conditions were analysed in terms of the relative rates of the reduction, oxidation, and hydrochlorination steps. New intermediates species were detected, such as $CuCl_2$ with chloride vacancy, the complexes of MCl_2-$CuCl_2$. This provides a significantly better understanding of the dynamic evolution of the active sites during the course of the reaction



IIA 5: The Next Step in Direct Activation of Lower Alkanes

The Team in 2019

Stian Svelle	UiO	IIA Leader, PhD supervisor, WP responsible (WP5.1-5.2-5.3)
Pablo Beato	Haldor Topsøe A/S	Industrial senior, Industry researcher (WP5.1-5.2-5.3),
Unni Olsbye	UiO	PhD supervisor (WP5.1-5.2)
Dimitrios Pappas	UiO	PhD student (WP5.1-5.2)
Karoline Kvande	UiO	Master student (WP5.1-5.2), PhD candidate (WP5.2)
Lars Fahl Lundegaard	Haldor Topsøe A/S	Industry researcher (WP5.1)
Aino Nielsen	Haldor Topsøe A/S	Industry researcher (WP5.1),
Martin R. N. Grøndahl	Haldor Topsøe A/S	Industry researcher (WP5.2),
Mia Bodenhoff	HTAS/DTU	Master student (WP 5.2)
Bjørnar Arstad	SINTEF	Researcher (WP5.3)

Motivation
Researchers at SINTEF, UiO and Haldor Topsøe AS join forces for developing new nanostructured catalyst materials. To this end, they try to reveal the mechanism of the direct conversion of lower alkanes to chemicals or liquid fuels over copper-doped zeolite catalysts.

Publication
Publications and conference contributions from IIA5 are listed in page 60.

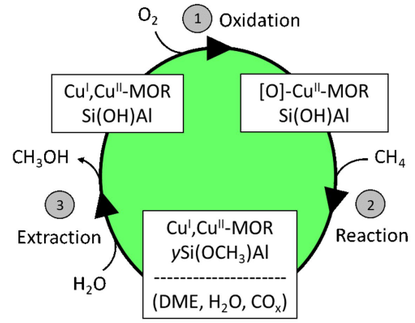
The low temperature activation and transformation of methane as well as other lower alkanes directly into valuable chemicals, such as methanol, is commonly considered "a dream reaction" due to its enormous industrial potential. Haldor Topsøe AS supplies essential technology to most existing routes but is monitoring potential extensions for the current portfolio and the application of zeotype materials.

A Generation Change

The year 2019 marked a milestone for the activities within IIA5. Dimitrios Pappas defended his PhD, a new PhD candidate, Karoline Kvande, has started her work, and a new postdoc will start in early 2020. Looking back, the activities within IIA5 during the first half of the Centre's existence have been tremendously successful. Starting from scratch, we have now moved to the research front within our topic, evidenced by the large number of publications and in particular the two papers in the high impact Journal of the American Chemical Society and a review article on the chemistry of Cu-zeolites in general published in Chemical Society Reviews. Apart from the great contributions of the candidates working on the project, a major contributing success factor has been the collaboration with the University of Turin. Through this collaboration, the IIA5 activities have gained access to extensive competence in characterization accumulated over decades. In supporting projects, we have carried out extensive quantum chemical calculations (yet to be published) and an effort has been made to evaluate process feasibility (Mia Bodenhoff, Master's thesis, DTU, Denmark). Looking ahead, we have identified several ambitious new objectives, and we are confident of making the second Centre period equally successful for IIA5!

2019 Research Highlight

As the 2019 research highlight, we would like to emphasize the publication *Zeolite surface methoxy groups as key intermediates in the stepwise conversion of methane to methanol* by Michael Dyballa, Knut Thorshaug, Dimitrios K. Pappas, Elisa Borfecchia, Karoline Kvande, Silvia Bordiga, Gloria Berlier, Andrea Lazzarini, Unni Olsbye, Pablo Beato, Stian Svelle and Bjørnar Arstad, published in ChemCat Chem 2019, 11, 5022-26.

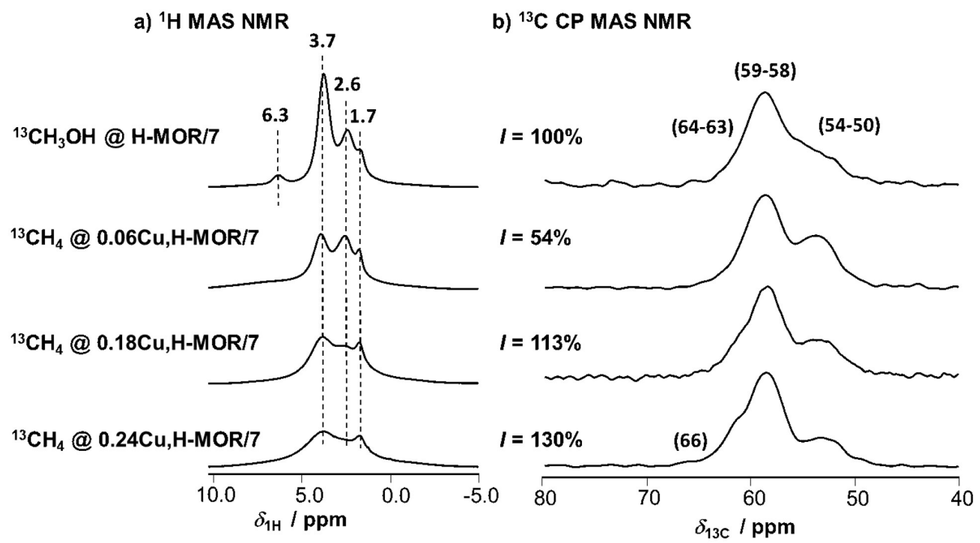


Pathway of the stepwise MTM conversion. CuII is present after oxidation (Step 1) but gets reduced to CuI by methane (Step 2). The reaction leads to the formation of stable surface methoxy groups (SMGs) and side products like water, COx and DME.

We are particularly pleased by this work, as it is a product of the collaboration among the entire IIA5 team, unlocking the full synergy of the team. Solid state NMR and sample activation and pretreatment was carried out at SINTEF. This was a milestone experiment for us, which required extensive method development. Thanks to iCSI-IIA5 activities, significant new competence has been built. Furthermore, measurements of methanol productivities have been done at UiO, Haldor Topsøe has prepared materials, and through the collaboration with the University of Turin, characterization has been carried out.

In this collaboration, we show that surface methoxy groups (SMGs) located at zeolite Brønsted sites are the stable key species to trap and store the methane oxidation products. We followed the reaction steps in situ via infrared spectroscopy and applied solid state NMR spectroscopy on copper mordenites after methane loading. The SMGs are identical to those formed on a copper-free reference zeolite after reaction with methanol. These SMGs react with water, methanol, or carbon monoxide to yield methanol, dimethyl ether and acetate. We find no evidence for stable SMGs directly at copper sites.

To conclude, we have identified two potential bottlenecks in the methane to methanol reaction, namely (1) the absolute amount of active copper species, tunable by a properly adjusted stoichiometry, and (2) the amount of Brønsted acid sites able to stabilize the SMG intermediate without overoxidation. Our finding explains why H-form mordenites outperform their Na-form analogues. This observation has general impact on any future process that tries to trap the intermediate methane oxidation product towards methanol.



1H and 13C solid state NMR demonstrating that the surface species (methoxy groups) formed during the conversion of methane to methanol over Cu-loaded zeolites are identical to those formed when methanol is adsorbed on a regular, Brønsted acidic

IIA 6: Generic Projects for Additional Industrial Synergies

The Team in 2019

Magnus Rønning	NTNU	IIA leader, PhD supervisor and WP responsible (WP6.1)
Anja Olafsen Sjåstad	UiO	WP responsible (WP6.2)
De Chen	NTNU	WP responsible (WP6.3)
Ragnar Fagerberg	SINTEF	WP responsible, researcher (WP6.4)
Torbjørn Gjervan	SINTEF	WP responsible, researcher (WP6.4)
Samuel K. Regli	NTNU	PhD candidate (WP6.1)
Hilde Johnsen Venvik	NTNU	PhD supervisor (WP6.1)
Martin Meuche	NTNU	Master student (WP6.1)
Edd A. Blekkan	NTNU	WP responsible and PhD supervisor (WP6.5)
Jia Yang	NTNU	Researcher and PhD supervisor (WP6.5)
Moses Mawanga	NTNU	PhD candidate (WP6.5)
Oleksii Ivashenko	UiO	Postdoctoral fellow (WP 6.2)
Pablo Beato	Haldor Topsøe	Industrial senior researcher (WP6.1)
David Waller	YARA	Industrial senior researcher (WP6.2)
Helmer Fjellvåg	UiO	Researcher (WP6.2)
Christine Pettersen	UiO	Master student (WP6.2)
Martin Jensen	UiO	PhD candidate, not iCSI (WP6.5)
Yanying Qi	NTNU	Postdoctoral fellow (WP6.3)
Terje Fuglerud	INOVYN	Industry senior researcher (WP6.1-WP6.3)
Kristin Bingen	Dynea	Industry senior researcher (WP6.3)
Kumar R. Rout	SINTEF	Researcher (WP6.3)
Rune Lødeng	SINTEF	Researcher (WP6.4)
Ingeborg Helene Svenum	SINTEF	Researcher (WP6.4)
Øystein Dahl	SINTEF	Researcher (WP6.4)
Anna Lind	SINTEF	Researcher (WP6.4)
Carlos Grande	SINTEF	Researcher (WP6.4)
Martin Fleissner Sunding	SINTEF	Researcher (WP6.4)
Mathieu Grandcolas	SINTEF	Researcher (WP6.4)
Otto Lunder	SINTEF	Researcher (WP6.4)
John Lein	SINTEF	Researcher (WP6.4)
Athanasios Chatzitakis	UiO	Researcher (WP6.4)

Motivation
Some iCSI work packages are allocated to research with the intention of moving the research to the forefront and providing methodological tools that can be applied in the industrial innovation areas IIA1-5. In particular, advanced spectroscopic and microscopic investigations under conditions highly relevant to industrial operation are targeted. Another effort is directed towards advancing atomistic and kinetic modelling of metals and oxides, as well as reactor modelling, to eventually enable an integrated, multiscale modelling approach.

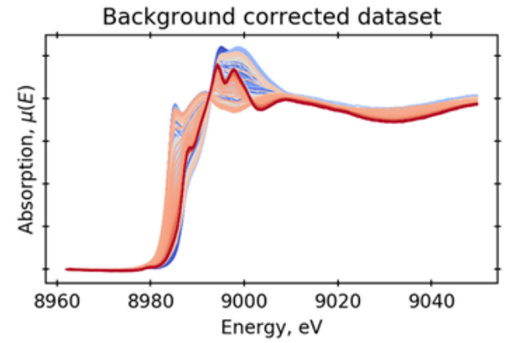
Publication
Publications and conference contributions from IIA6 are listed on page 60.

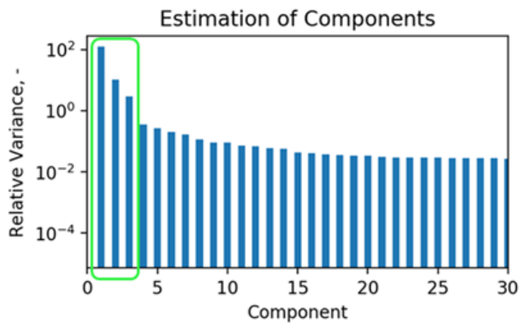
Advanced Operando Characterization of Heterogeneous Catalysts for Sustainable Process Industries

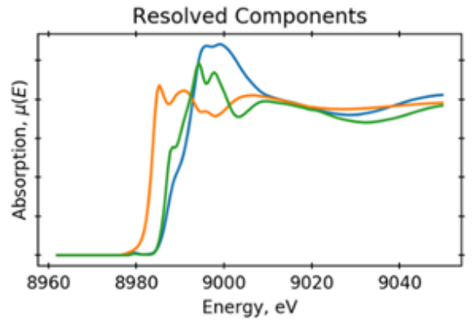
PhD Project, WP6.1
This work package is investigating heterogeneous catalysts during operation at industrially relevant conditions and developing the necessary data analysis tools as needed. In order to link structural properties of the material with catalytic activity during reaction, we apply spectroscopy (Infrared, X-ray, UV-Vis) in-house and at synchrotrons. We have synergies with four out of the five other industrial innovation areas within iCSI and collaborations within KinCat (Fe-based Fischer-Tropsch synthesis to olefins from renewable feedstocks and selective catalytic reduction of NO by ammonia over Cu-based catalysts) and with SUNCAT at Stanford University.

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

The activity this year has focused particularly on multivariate statistical analysis of in situ and operando X-ray Absorption Spectroscopy data. The increasingly larger datasets associated with studies of catalysts at work, often combining several characterization techniques, call for automated procedures for analysing a large number of spectra simultaneously. The work has made strides in finding previously unknown intermediate components in XAS spectra of e.g. oxychlorination catalysts, and our aim is to be able to identify the chemical nature of such species by combining multivariate statistical analysis and our chemical knowledge of the catalyst system.







The figures show changes in Cu spectra in an operando X-ray absorption spectroscopy dataset during oxychlorination. The blue bars show the estimated number of components from singular value decomposition, and the three resolved Cu components from multivariate statistical analysis are displayed in the lower figure.

Advanced Synthesis and Characterization – Novel Thin Film Preparation and Reactor STM

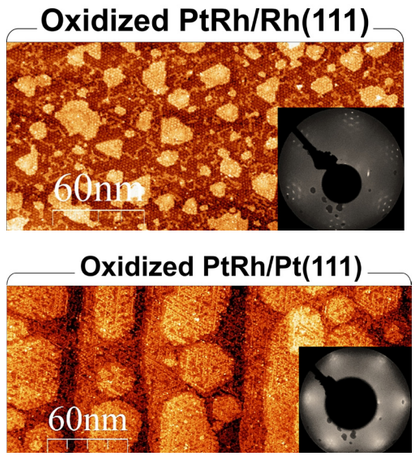
Postdoctoral Fellowship, WP6.2
In this work package we are developing nanostructured surfaces, which act as model catalysts relevant for industrial processes. The obtained model catalysts are utilized in surface sensitive operando studies by means of Reactor STM-MS and Near Ambient-Pressure (NAP) XPS-MS. We are currently focusing on catalytic ammonia oxidation at intermediate temperatures (200-400 °C) for environmental applications. Since Pt-Rh gauzes are used as catalysts for ammonia oxidation for nitric acid production, this bimetallic alloy is also considered for the ammonia slip process.

Three activities are ongoing in parallel to reveal the role of Rh in the PtRh alloy at ammonia slip conditions:

1. Understanding of alloying of PtRh surfaces based on Pt(111) and Rh(111) single crystals

2. Observing oxidation of alloyed surfaces using in situ STM and NAP XPS

3. Capturing ammonia oxidation live with high pressure Reactor STM and NAP XPS



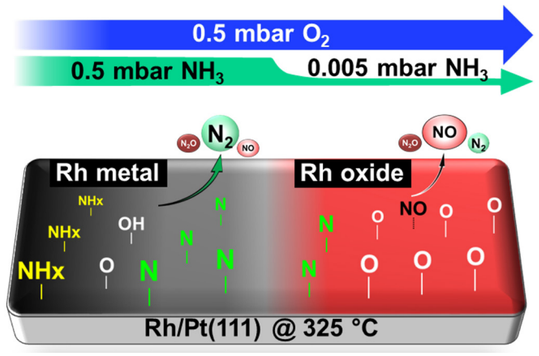
UHV STM of oxidized PtRh alloy prepared on Rh(111) and Pt(111) surfaces. Low energy electron diffraction images in the insets show long and short range ordered structures observed in each case; Activity 2.

With the aim of understanding the structure and morphology of PtRh alloys, we previously constructed a roadmap for alloy preparation on the Pt(111) surface. In 2019 a complementary work on Rh(111) was initiated together with Christine Pettersen. From the comparison of PtRh/Pt(111) and PtRh/Rh(111), it follows that they exhibit distinct surface morphology, which in future can be used to improve catalytic performance.

To explain the behaviour of PtRh alloys in ammonia oxidation conditions, the obtained surfaces were oxidized in various conditions to identify surface structures possible in the presence of O_2. The lower part of the figure above highlights the differences in surface structures of oxidized PtRh prepared on Pt(111) and Rh(111) crystals.

Finally, the NAP XPS data obtained at MAXIV in collaboration with international partners at Lund University have been analysed and provide the first operando insights on how the surface species present on PtRh/Pt(111) are driving product distribution during ammonia oxidation. This activity has synergies with IIA1 (21st Century Ammonia Oxidation and Nitric Acid Technology Development).

All the experimental results collected to date form a solid basis for further operando studies of PtRh/Rh(111) at the MAXIV and PtRh/Al_2O_3/NiAl(110) at the SOLEIL synchrotrons scheduled in 2020.

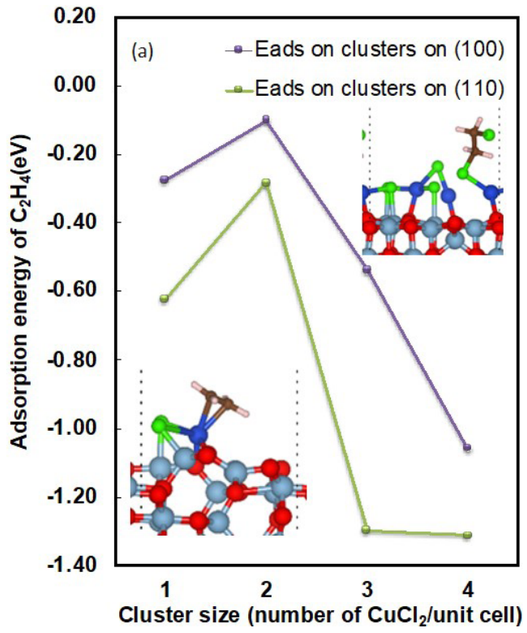


Schematic drawing on the right shows summary of surface oxidation state and adsorbates present in each case.

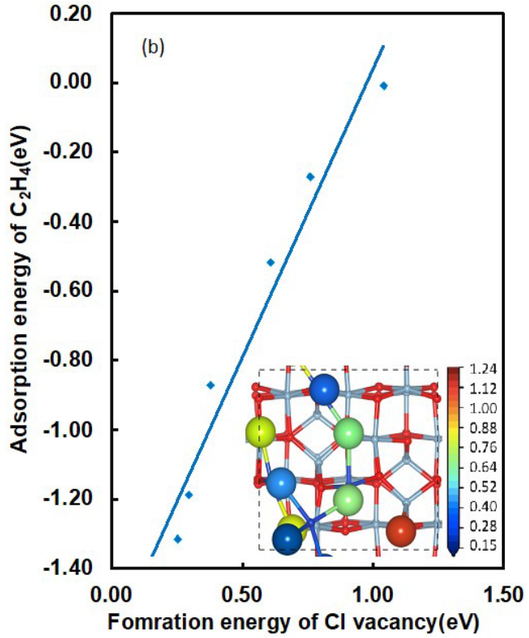
Reaction Mechanism Investigation by Combined DFT Calculations and Microkinetic Modelling

Postdoctoral Fellowship WP6.3
Developing new catalysts or improving existing catalysts depends on a better understanding of the reaction mechanism on the catalyst surface and the relationship between the catalyst properties and performance. The Density Functional Theory (DFT) calculation has been carried out to describe surface reactions and provide so-called descriptors of catalytic activity and selectivity to be able to tailor catalysts atom by atom. Microkinetic modelling is utilized to investigate the reaction mechanism and predict information about surface coverages and relative rates of various elementary steps under reaction conditions. By developing this methodology, the project has enabled us to bridge the gap from the atomic level to kinetic analysis at the macro-scale.

The approach is currently being employed in reaction systems of ethylene oxychlorination and methanol oxidation to formaldehyde. An understanding of mechanisms and processes on many levels has been gained, including the atomic insights of the active sites and elementary steps of the reactions, understanding the details of the atomic structure of the active sites of $CuCl_2$, the interaction between the $CuCl_2$ and the alumina surfaces, as well as the effects of alkali and/or rare earth promoters on the $CuCl_2$ reduction and CuCl oxidation in ethylene oxychlorination.



Cluster-Size-dependent Eads,C_2H_4 and inserted adsorption configurations at $CuCl_2$ and $(CuCl_2)_3$/γ-Al_2O_3 (110).



Adsorption energy of ethylene as a function of formation energy of Cl vacancy on $(CuCl_2)_4$ /γ-Al_2O_3 (110) and the mapping of the ΔeV of all the Cl atoms on $(CuCl_2)_4$ / γ-Al_2O_3 (inserted figure).

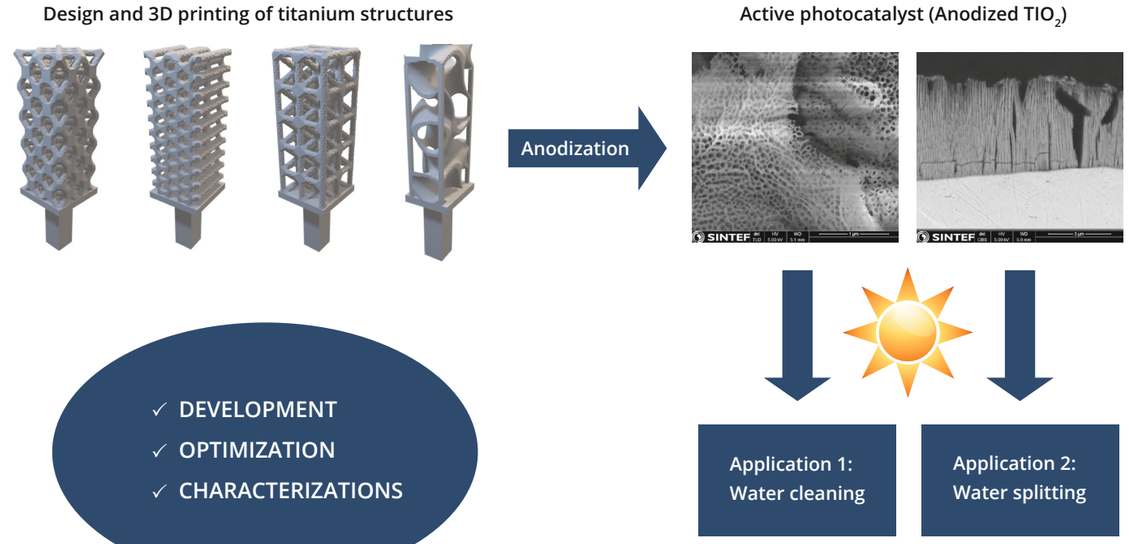
Anodization of 3D Printed Titanium for Photocatalysis (PHOTO-3D)

SINTEF Work, WP 6.4:
Titanium dioxide (TiO_2) is a common material for photocatalysis due to its high efficiency, low cost, chemical inertness and high photostability. Highly ordered, vertically oriented arrays of TiO_2 nanotubes can be prepared on a Ti substrate by electrochemical anodization. The use of TiO_2 nanotubes generally offers a larger surface area compared to nanoparticles, as well as channels for enhanced electron transfer. The TiO_2 nanotubes also have high adsorption capacity and efficient charge separation can be achieved, which reduces the efficiency loss due to recombination of photogenerated electrons and holes.

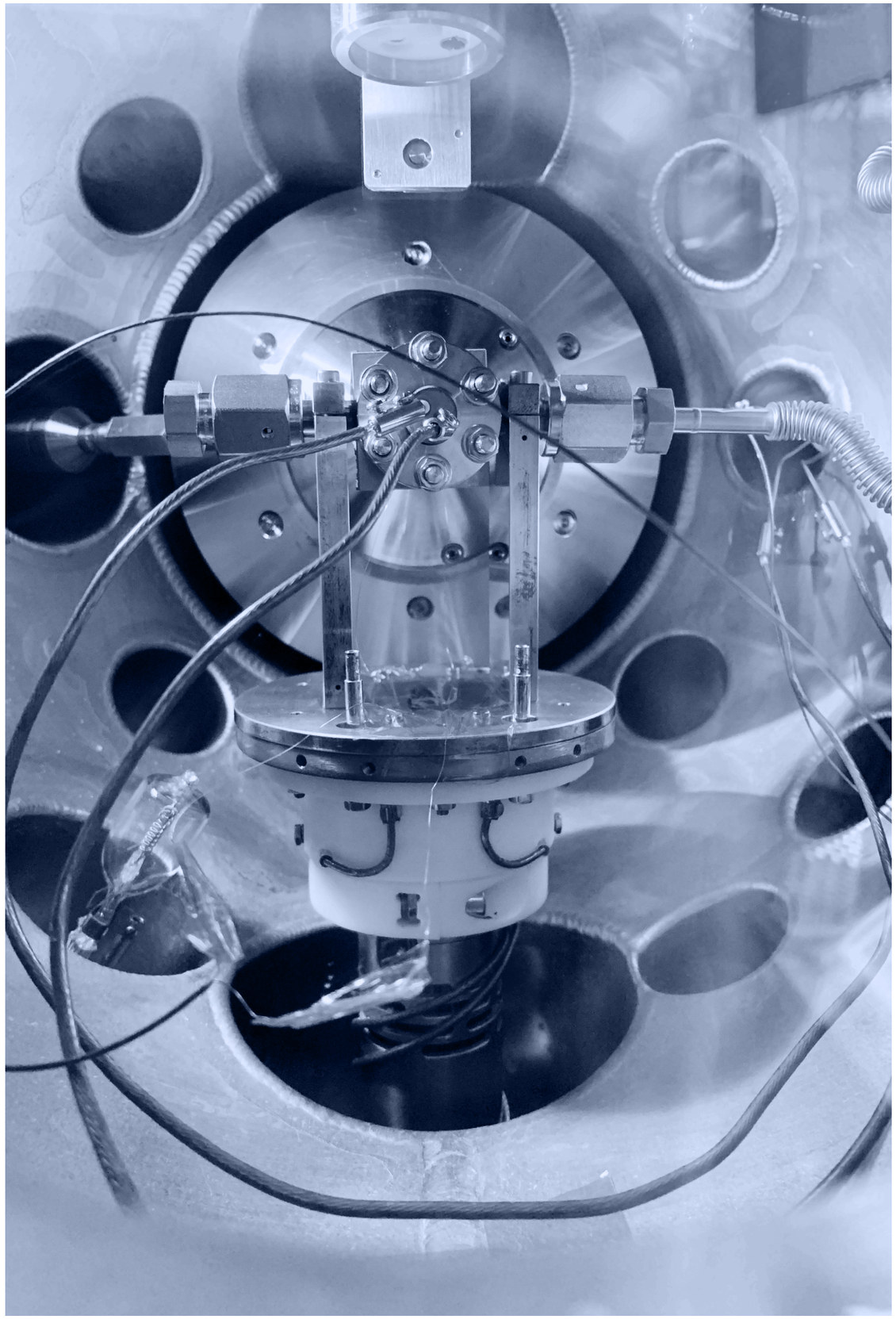
The main idea of this project is to produce an advanced photocatalyst by combining the concept of 3D printing and anodization of titanium (Ti), and to prove its activity towards water cleaning and water splitting under solar illumination (figure below).

Many literature reports are based on anodization of Ti foils, whereas here we use 3D printed Ti structures as substrates for the anodization. The benefit of using 3D printing in the design of a photocatalytic reactor or electrode is that the structure can be computer-designed to satisfy multiple criteria. We can optimize the 3D structures of the photocatalytic reactors to substantially increase the surface area/volume accessible to the light, compared to what is possible with conventional photocatalytic reactors and yielding a crucial improvement in the efficiency of the photocatalysts.

The figure below illustrates some selected electrode designs that have been successfully 3D printed and anodized. When working with 3D printed materials, factors such as material roughness and alloying elements, as well as the lower accessibility of the surface to be anodized, affect the anodization process. This requires the development of new photocatalyst preparation methodologies. The next step in this project is to test these photocatalysts in wastewater treatment and water splitting.



Schematic illustration of the project's workflow, from designing, optimizing and printing of the 3D structures to anodization of TiO_2 nanotubes onto the 3D structures to testing of the prepared photocatalysts in the two selected applications.

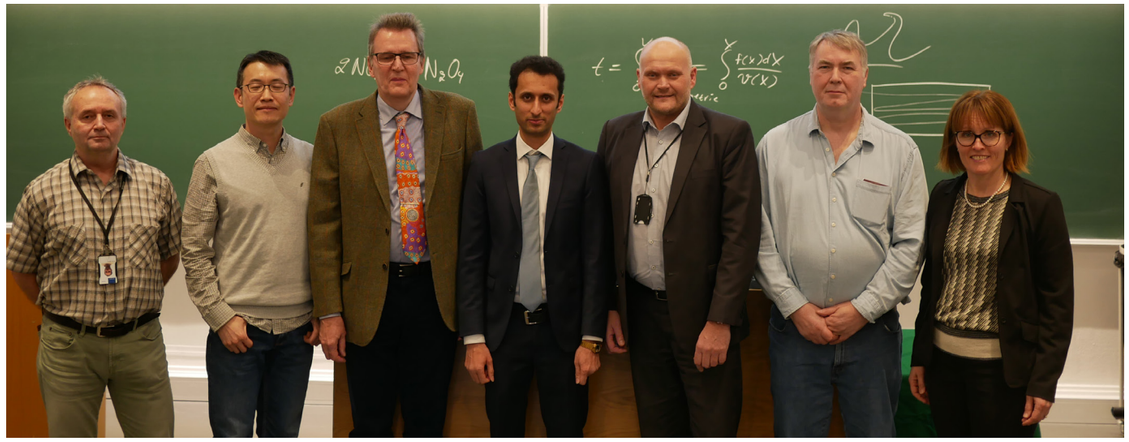


Two new PhDs

Candidate: Ata ul Rauf Salman
Date of defense: December 6, 2019
Title of thesis: Catalytic oxidation of NO to NO2 for nitric acid production
Public trial lecture: Nitrogen fixation beyond Haber-Bosch – recent developments in heterogeneous catalysis and electrocatalysis

The Committee:
First opponent: Professor Lars J. Pettersson, KTH, Sweden
Second opponent: Dr. Sang Baek Shin, Yara Technology Centre, Porsgrunn
Administrator: Professor Hilde J Venvik, NTNU

Supervisor: Professor Magnus Rønning, NTNU
Co-supervisors: Rune Lødeng, SINTEF, Bjørn C. Enger, SINTEF
iCSI project: 21st century Ammonia Oxidation and Nitric Acid technology development.
Industry partner: YARA
Current Position: Equinor, Herøya



Ata ul Rauf Salman (in the middle) surrounded by opponents and supervisors

The current work aims to replace the homogenous reaction in the Ostwald process from 1902 with a more compact heterogeneous catalytic process for producing nitric acid. This is done by finding efficient catalysts for oxidation of NO to NO_2, at conditions relevant to nitric acid plants, enabling significant process intensification of the production plant. Additionally, the aim was to gain fundamental understanding of reaction kinetics and the mechanism of oxidation of NO over promising catalysts. Further details in the current work and results are described on page 31 under the Scientific Activities in IIA1.

Candidate: Dimitrios Papas
Date of defense: December 13, 2019
Title of thesis: Direct methane to methanol conversion over Cu-exchanged zeolites: Building structure - activity relationships
Public trial lecture: Overview of catalysts for methanol synthesis from carbon dioxide – structure to property relations

The Committee:
First opponent: Professor Jeroen A. van Bokhoven, ETH Zürich, Switzerland
Second opponent: Assistant Professor Chris Paolucci, University of Virginia
Administrator: Professor Ola Nilsen, UiO

Supervisor: Professor Stian Svelle, UiO
Co-supervisors: Pablo Beato, Haldor Topsøe, Professor Unni Olsbye, UiO
iCSI project: The next step in direct activation of lower alkanes
Industry partner: Haldor Topsøe AS
Current Position: CorrsTek Membrane Science, Oslo

Celebration of Dimitrios Papas' approved PhD defense (Dimitrios to the right).

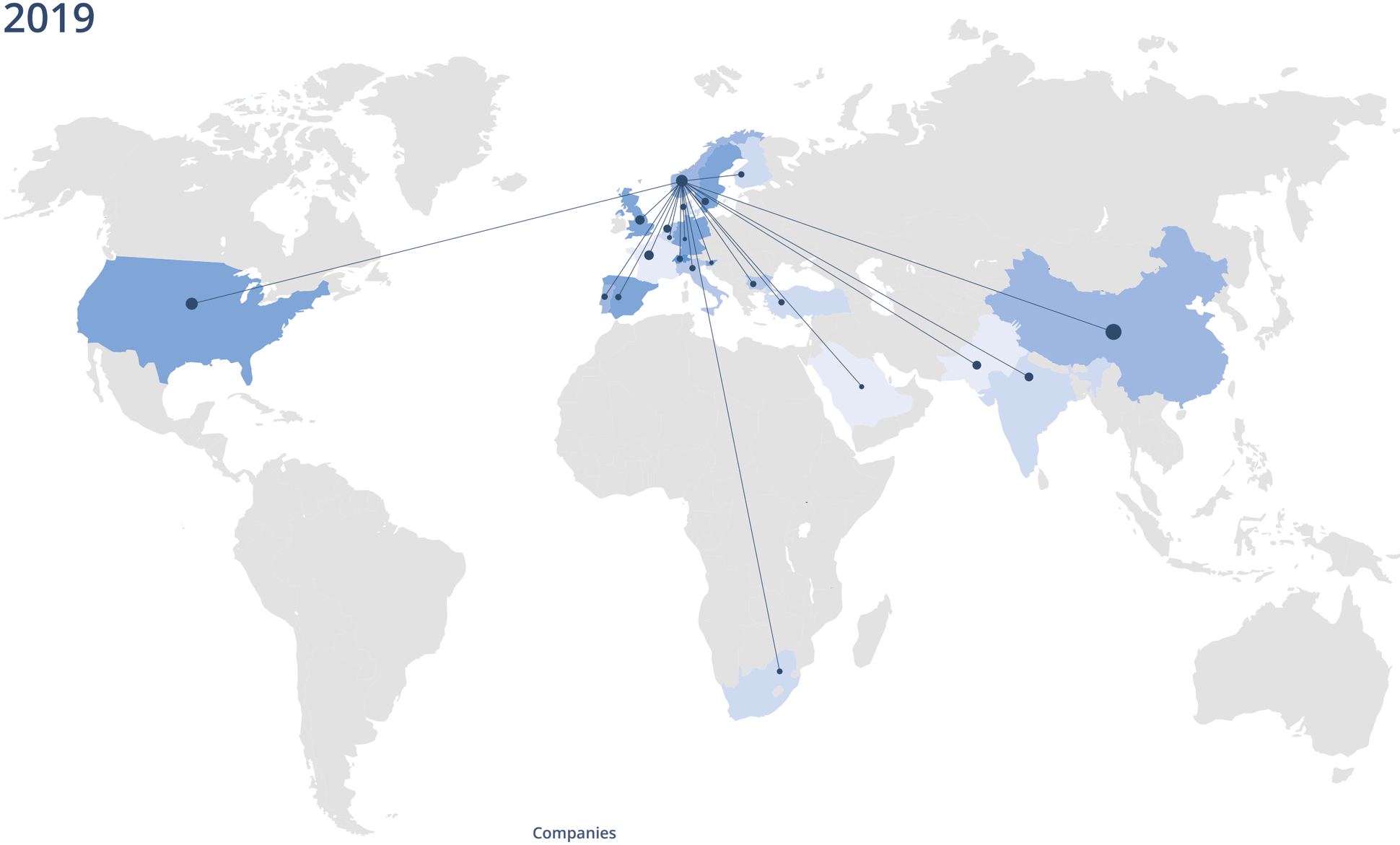
The direct conversion of methane to added value chemicals, in particular methanol, is a topic intensively researched by the academia and the industry due to large environmental and economic benefits. Such a process could provide an alternative to the capital- and energy-intensive syngas route for methanol synthesis as well as contribute in reducing methane flaring. To this end, different catalytic processes have been investigated over the past decades.

In this thesis, copper-loaded zeolites are investigated for the direct conversion of methane to methanol. Zeolites, which have numerous applications in catalysis, are microporous aluminosilicates with defined structures able to host active metal centres. The conversion of methane to methanol over copper-exchanged zeolites is a stepwise process. Initially the material is pre-treated in oxygen at high temperature, then methane activation takes place at a lower temperature, and finally methanol is extracted by hydrolysis of the stabilized intermediate. Different copper-exchanged zeolites have been investigated, including chabazite, ferrierite and mordenite, aiming to understand the mechanism of the conversion as well as the fundamental properties of the materials. These are achieved by combining activity measurements with in-situ and operando characterization techniques and establishing structure activity relationships.

Internationalization 2019

iCSI is an attractive project for international researchers. The 89 master students, PhD candidates, postdocs and guest researchers within or affiliated with iCSI represent 22 countries. Non-Norwegians make up 64% of this group of employees.

In July 2019, SINTEF researcher Ingeborg-Helene Svenum returned after one year as a guest researcher in the group of Professor Manos Mavrikakis at the University of Wisconsin-Madison College of Engineering.



Overview of international collaborations:

Universities and Institutes

- *Aalto University, Finland*
- *Anna University, Department of Chemistry, Chennai, India*
- *Bulgarian academy of Science, Bulgaria*
- *Cardiff University, United Kingdom*
- *Chalmers University of Technology, Sweden*
- *CNR, Italy*
- *Dalian Institute of Chemical Physics, Chinese Academy of Sciences, China*
- *Delft University of Technology, Netherlands*
- *Durham University, United Kingdom*
- *East China University of Science and Technology, China*
- *ECN, Netherlands*
- *European Research Institute of Catalysis A.I.S.B.L., Belgium*
- *Ghent University, Belgium*
- *Institut de Recherches sur la Catalyse et l'Environnement de Lyon, CNRS, France*
- *Instituto Nacional del Carbón, INCAR-CSIC, IMDEA Energy Institute, Spain.*
- *Karlsruhe Institute of Technology – KIT, Germany*
- *KAUST, Saudi Arabia*
- *Kemijski Institut (NIC), Slovenia*
- *Leiden University, Netherlands*
- *Linné University, Sweden*
- *Lund University, Sweden*
- *MAX-IV Laboratory, Lund, Sweden*
- *National University of Science and Technology, Pakistan*
- *Paul Sherrer Institut, Schweiz*
- *Polytech Sorbonne, France*
- *Politecnico di Milano, Italy*
- *Royal Institute of Technology (KTH), Sweden*
- *School of Chemistry and Chemical Engineering, Shanghai Jiao Tong University, China*
- *Shanghai Institute of Applied Physics, China*
- *Shanxi Institute of Coal Chemistry, Chinese Academy of Sciences, (ICC), China*
- *Sorbonne University, France*
- *Stanford University, California, USA*
- *Swiss-Norwegian Beamlines at ESRF, France*
- *Technical University of Denmark, Denmark*
- *Technische Universiteit Eindhoven; Netherlands*
- *Tianjin University, China*
- *University of California, Berkeley, USA*
- *University of Cape Town, South Africa*
- *University of Duisburg-Essen, Germany*
- *University of Porto, Portugal*
- *University of Sheffield, United Kingdom*
- *University of Wisconsin-Madison, USA*
- *University of Torino, Italy*
- *Utrecht University, Netherlands*

Companies

- *Arkema France SA; France*
- *Asociacion Espanol de NormalizacionA, Spain*
- *B.T.G. BV, Netherlands*
- *Borealis, Austria*
- *BTG-BTL, Belgium*
- *C2P2, Lyon (CNRS)*
- *Compania Espanola de Petroleos, Spain*
- *DOW chemicals*
- *ENI S.p.a., Italy*
- *Fundacio EURECAT, Spain*
- *GE Healthcare, Norway*
- *Haldor Topsøe AS, Denmark*
- *Johnson Matthey, UK*
- *Linde, Germany*
- *Perstorp AB, Sweden*
- *Processi Innovativi SRL, Italy*
- *ProfMOF AS, Norway*
- *Repsol SA, Spain*
- *SABIC, Saudi Arabia*
- *SICAT Sarl, France*
- *ST1, Finland*
- *Steeper, Denmark*
- *Strane Innovations SAS, France*
- *Tata Steel UK Limited*
- *Turkiye Petrol Rafinerileri Anonim Sirketi (Tüpras),*
- *UOP LLC*
- *Velocys, USA*
- *VTT, Finland*

European research projects

WASTE2ROAD -Biofuels from WASTE TO ROAD transport. (Coordinator). H2020-LC-SC3-RES-21-2018: iCSI Partners involved: SINTEF. Duration: 2018-2022.

Pulp and Fuel - Pulp and Paper Industry Wastes to Fuel. H2020-LC-SC3-RES-21-2018. iCSI Partners involved: SINTEF. Duration: 2018-2022.

Bizeolcat - Bifunctional zeolite-based catalysts for sustainable hydrocarbon transformation. Horizon 2020 CE-NMBP-24-2018 - iCSI Partners involved: SINTEF, UiO. Duration: 2019-2022.

BIKE - BImetallic Catalysts Knowledge-based development for Energy applications. Horizon 2020 MSCA-ITN: iCSI Partners involved: NTNU. Duration: 2019-2023.

C123 - Methane oxidative conversion and hydroformylation to propylene. (Coordinator). Horizon 2020 CE-NMBP-24-2018. iCSI Partners involved: SINTEF. Duration: 2019-2023.

COZMOS - CO2 hydrogenation to light hydrocarbons (UiO coordinator). H2020-LC-SC3-RIA & H2020-LC-SC3-2018-NZE-CC: UiO, SINTEF, Topsøe: Status: 2019-2023.

4Refinery - Scenarios for integration of bio-liquids in existing REFINERY processes. H2020-LCE-2016-RES-CCS-RIA, iCSI Partners involved: SINTEF. Duration: 2017 - 21

CARMOF – New process for efficient CO2 capture by innovative adsorbents based on modified carbon nanotubes and MOF materials. H2020-NMBP-20-2017, iCSI Partners involved: SINTEF. Duration: 2018 –21

Research Council of Norway (RCN) projects with international collaborations

EmX 2025 - an R&D base for reduced exhaust emissions in the Norwegian marine transportation sector. TRANSPORT 2025 Researcher project (246862). iCSI Partners involved: NTNU/ SINTEF. Duration 2015-2019. International partner: Chalmers University of Technology, Sweden.

GAFT Gasification and FT-Synthesis of Lignocellulosic Feedstocks, ENERGIX Knowledge-Building Project for Industry (280903). iCSI Partner involved: SINTEF. Duration: 2015-2019.

Bio4Fuels - Norwegian Centre for Sustainable Bio-based Fuels and Energy. Centre for Environment-friendly Energy Research (FME, 257622), iCSI Partners involved: SINTEF/ NTNU. Duration: 2016 - 2024

MBCL - Moving Bed Carbonate Looping, CLIMIT-supported (Gassnova), Owned by FTG (Fjell Technology Group), iCSI Partners involved: NTNU, SINTEF, International partner: Southeast University, China, Duration 2017 -202x

H_2MemX - Enabling ultrathin Pd based membranes through surface chemistry diagnostics and control. ENERGIX Researcher project (280903). iCSI Partners involved: NTNU, SINTEF. Duration 2018 – 2021. International partner: Lund University/MAX IV, Sweden.

NanoCat4Fuels - Production of JP-8 Range Fuels and Chemicals from Pyrolysis Bio-Oil using Nanostructured Catalyst, Indo-Norwegian initiative on renewable fuels and chemicals within the Bionær and EnergiX work program, iCSI Partners involved: SINTEF, International partner: Anna University, Department of Chemistry, Chennai, India Duration: 2018 – 2021

Accounts 2019

Table 1 summarizes the costs in 2019 and the total budget for the period of the Centre after revision in January 2020. The different cost codes concern respectively:

- **NTNU costs in Payroll and indirect expenses**
- **Other research partners (SINTEF and UiO) in Procurement of R&D services**
- **Equipment code includes rent of research equipment acquired to serve needs for the SFI**
- **Other operating expenses regroups mainly research at industrial partners**

Cost code	Costs 2019, kNOK	2015-2023 Total budget
Payroll and indirect expenses	7 792	59 413
Procurement of R&D services	11 169	92 378
Equipment	902	7 305
Other operating expenses	4 917	34 078
Totals	**24 780**	**193 174**

Table 2 presents the cost and financing per partner. The industrial partners are Yara ASA, Dynea AS, INOVYN AS, KA. Rasmussen AS and Haldor Topsøe A/S.

Cost and Financing per partner	2019 Accounts		2015-2023 Total budget	
Partner	**Costs**	**Financing**	**Costs**	**Financing**
NTNU	10 137	2 488	75 252	27 074
University of Oslo	6 378	2 158	48 877	12 700
SINTEF	4 792	1 471	43 501	7 858
Industrial partners	3 475	6 474	25 543	49 543
Research Council of Norway	-	12 191	-	96 000
Totals	**24 780**	**24 780**	**193 174**	**193 174**

Table 3 presents the costs per Industrial Innovation Area (IIA). The iCSI Management and administration include the overall administration of the Centre (Director, Coordinator and Economy advisor, meetings, seminars, SAC compensation and expenses, international exchange funding).

Industrial Innovation Area (IIA)	Costs 2019	2015-2023 Total budget
IIA1 21st century Nitric Acid technology development	3 783	36 648
IIA2 New NOx abatement technologies	621	7 574
IIA3 Frontier formalin technology development	2 800	22 907
IIA4 PVC Value Chain	4 692	31 027
IIA5 The next step in direct activation of methane	4 067	34 492
IIA6 Generic projects	6 980	36 323
IIA7 2020 Catalysis	-	7 495
iCSI Management and administration	1 838	16 708
Totals	**24 780**	**193 174**

**In all tables above values appear in 1000 NOK (as per January 2020 10 NOK are equivalent to 1€)*

Education

Postdoctoral fellows with financial support from iCSI in 2019

Yanying Qi	NTNU	China	2016-2020	F	IIA6
Oleksii Ivashenko	UiO	Ukraine	2016-2020	M	IIA1/IIA6
Yalan Wang	NTNU	China	2019-2021	F	IIA4

Yalan Wang

One new postdoctoral fellow was welcomed in 2019, Yalan Wang joined iCSI in May. She finalized her PhD in the Catalysis group at Department og Chemical Engineering, NTNU, in March 2019.

2019 PhD candidates with financial support from iCSI

Ata ul Rauf Salman	NTNU	Pakistan	2015 - 2019	M	IIA1
Dimitrios Pappas	UiO	Greece	2016 - 2019	M	IIA5
Endre Fenes[1)]	NTNU	Norway	2015 - 2020	M	IIA4
Samuel Regli	NTNU	Switzerland	2016 - 2020	M	IIA6
Stine Lervold	NTNU	Norway	2016 - 2020	F	IIA3
Asbjørn Slagtern Fjellvåg	UiO	Norway	2016 - 2020	M	IIA1
Hongfei Ma	NTNU	China	2017 - 2020	M	IIA4
Moses Mawanga	NTNU	Uganda	2018 - 2021	M	IIA6
Karoline Kvande	UiO	Norway	2019 - 2022	F	IIA5
Julie Hessevik	UiO	Norway	2019 - 2023	F	IIA1

1) Endre Fenes left iCSI in 2019 for a job in the industry, and his defense is delayed.

2019 PhD candidates in iCSI with financial support from other sources,

Bjørkedal , Ole H.	NTNU	Norway	2016-2020	M	Selective catalytic reduction (SCR) of NO_X emissions in maritime transport.
Muhammad Zubair	NTNU	Pakistan	2017-2020	M	Enhanced visible light adsorption TiO_2 based catalysts for photocatalytic H_2 production
Martina Cazzolaro	NTNU	Italy	2017-2020	F	Cu/CNF for selective hydrogenation of hydroxyacetone to 1,2-propanediol
Joakim Tafjord	NTNU	Norway	2017-2020	M	Iron-based Fischer Tropsch synthesis based on renewable feedstocks
Jianyu Ma	NTNU	China	2017-2020	M	Chemical looping desulphurization
Daniel Skodvin	NTNU	Norway	2017-2020	M	Carbon Nanomaterial-Ionic Liquid Hybrid for Ultrahigh Energy Supercapacitor
Mario Ernesto Casa-legno	NTNU	Spain	2018-2022	M	Catalyst for onboard hydrogen generation from bioethanol
Jibin Antony	NTNU	India	2018-2021	M	Nanostructured hybrid catalysts for photocatalytic applications
Ask Lysne	NTNU	Norway	2019-2022	M	Staging and Multiple Hydrogen Feed of Biomass to Fischer-Tropsch Fuel Synthe-sis
Dumitrita Spinu	NTNU	Romania	2019-2022	F	Low temperature CO_2 capture
Junbo Yu	NTNU	China	2019-2022	M	Hydrogen membrane separation technology
Magnus Mortén	UiO	Norway	2015-2019	M	Acid strength of metal substituted aluminium phosphates
Emil S. Gutterød	UiO	Norway	2016-2019	M	On the kinetics and confinement effects of partial methane oxidation over Cu-MOFs
Volodymyr Levchenko	UiO	Ukraine	2016-2020	M	Au-based catalysts for C-C and C-X couplings
Giuseppe Rotunno	UiO	Italy	2016-2019	M	Autocatalysis and chiral amplification in metal organic frameworks
Mustafa Kømurcu	UiO	Norway	2017-2020	M	Ethene oligomerization
Martin Jensen	UiO	Norway	2018-2022	M	Materials for catalytic oxidation of ammonia

2019 International exchange PhD candidates and visiting researchers, NTNU and UiO

Weixin Qian	East China University of Science and Technology	M	8 mths	The mechanistic and kinetic study of CO and CO2 hydrogenation to chemicals and fuel
Xiaoli Yang	Dalian Institute of Chemical Physics	F	8 mths	The conversion of syngas to liquid hydrocarbons with OX-ZEO process
Nianju Hou	Tianjin University	F	12 mths	Ethanol fuel cells and also the ORR catalysts for fuel cells.
Gang Wang	East China University of Science and Technology	M	3 mths	Oxidation of propene to propene oxide with gold catalyst
Wenzhao Fu	East China University of Science and Technology	M	2 mths	Redox catalytic cycle of VOC oxidation and ethylene epoxidation
Hao Zhang	Shanghai Institute of Applied Physics	M	2 mths	XAS study of nanoclusters in electrochemical reaction
Silvia Bordiga	University of Turin	F	1 mth	Spectroscopic investigations of porous materials
Tommaso Selleri	Department of Energy, Politecnico di Milano	M	1 mth	Operando UV-vis measurement on Cu-CHA catalysts
Lukasz Kuterasinski	Jerzy Haber Inst.of Cat. and Surf. Chemistry, Polish Ac.of Sciences	M	2 weeks	Conversion of methanol to hydrocarbons over hierarchical zeolite catalysts

2019 Postdoctoral researchers working on projects in iCSI with financial support from other sources, NTNU and UiO

Chen, Qingjun	NTNU	China	2015- 2019	M	First principles modeling of Co based FTS catalysts
Jørgen Svendby	NTNU	Norway	2017- 2019	M	Designing new renewable nanostructured electrode and membrane materials for direct alkaline ethanol fuel cell
Xiang Feng	NTNU	China	2017-2019	M	catalytic pyrolysis of biomass towards olefin production
Strømsheim, Marie Døvre	NTNU	Norway	2018- 2020	F	surface chemistry and segregation phenomena of Pdalloy membranes
Gavrilovic Ljubisa	NTNU	Serbia	2018 - 2020	M	Bio Fischer-Tropsch (BioFT)Staging and Multiple Hydrogen. Feed of Biomass to Fischer-Tropsch Fuel Synthesis
Zhenping Cai	NTNU	China	2018- 2020	M	conversion of lignocellulosic wastes into biofuels and bioplastics
Ainara Moral Larrasoana	NTNU	Spain	2018 - 2020	F	MBCL project
Yuanwei Zhang	NTNU	China	2018 - 2019	M	MBCL project – simulation work
Suresh Balasingam	NTNU	India	2018 - 2020	M	Energy storage by high energy supercapacitors
Irene Panela Herrero	UiO-Katalyse	Spain	2017-2020	F	Production of aromatics from methanol via metal-exchanged zeolites
Andrea Lazzarini	UiO-Katalyse	Italy	2017-2019	M	Detailed characterization of complexes and nanostructured materials

Spring 2019 Master thesis in Chemical engineering (NTNU) or Chemistry (UiO) associated with iCSI

Galina T. Yavasheva	Bulgaria	F	Synthesis and characterization of bimetallic nanoparticles for selective catalytic conversion of ammonia
Mia Bodenhoff1)	Denmark	F	Combined experimental, spectroscopic, and theoretical mechanistic investigations
Dumitrita Spinu	Moldavia	F	Production of Fuels from Lignin by Fast Hydropyrolysis with Coupled Catalytic Upgrading
Minadir Saracevic	Norway	M	Efficient catalysts for achieving NO /NO_2 equilibrium
Martin Meuche	Norway	M	Perovskite catalysts study by MS and FTIR
Lisa L. Landfall	Norway	F	New catalysts for low-temperature selective catalytic reduction (SCR)
Kristiane S. Oftebro	Norway	F	Photocatalytic Ammonia Synthesis
Erik A. Jørgensen	Norway	M	Fischer-Tropsch Synthesis: Conversion of Bio-Syngas to Hydrocarbons
Abdul R. Toutounji	Lebanon	M	Carbon formation and catalysis in the conversion of methyl chloride and silicon into dimethyldichlorosilane
Fatemeh Khodadady	Qatar	F	process design and evaluation of CO_2 capture on solid sorbents
Siyu Wang	China	F	Synthesis of low temperature sorbents for CO_2 capture
Tho Ba Tran	Norway	M	Kinetic study of ethylene oxychlorination on promoted $CuCl_2$/Al_2O_3 catalysts

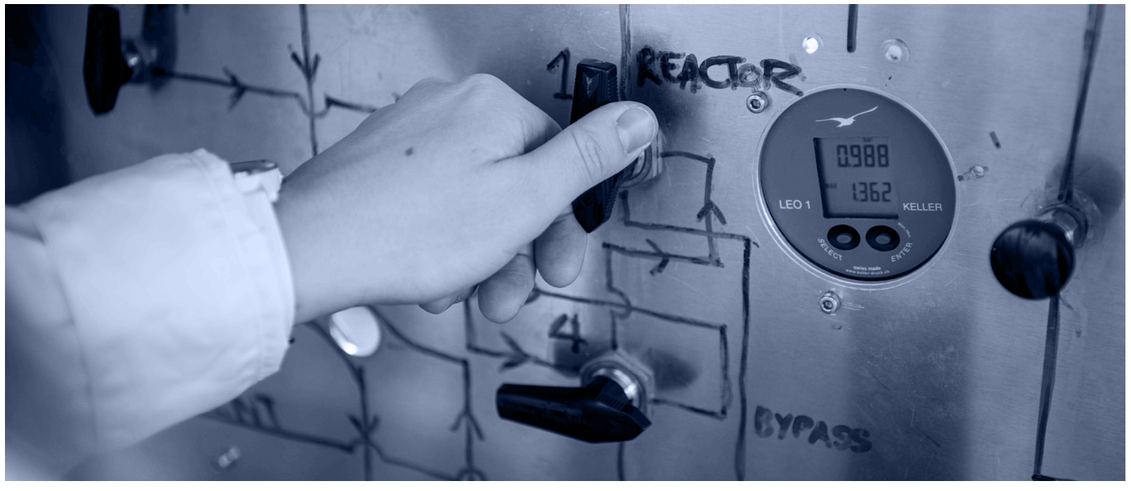
1) Mia Bodenhoff was a student at DTU, performing her master in collaboration with Haldor Topsøe and IIA5

2019 International exchange bachelor or master students, NTNU and UiO

Angelo Bellia	Italy	M	Synthesis of titanium free mordenite zeolites for the direct conversion of methane to methanol
Alizée Bataille	France	F	Production of H_2 using red mud
Christian Maier	Germany	M	Catalytic methane abatement for natural gas engines
Asma Hayoune	Algeria	F	Photocatalytic H_2 production
Henrik Schuster	Germany	M	Catalytic Methane Abatement for Natural Gas Engines
Constance Debionne	France	F	Polymers Assisted Preparation of Iron based Fischer-Tropsch Catalysts for biomass to fuel
Philip Walter Putze	Germany	M	Methodology Development for the Characterization of Contact Mass in the Direct Process

Autumn 2019 Specialization projects students

Ingvill Andrea Røed	Norway	F	Low temperature selective hydrogenation using noble metal catalysts
Petter Tingelstad	Norway	M	Biomass conversion to fuels / Oxidation, autoclave, catalyst
Kishore Rajendran	India	M	Biomass conversion to chemical / Fixed bed reactor, ethanol
Oscar I. Encinas	Spain	M	High temperature CO_2 capture / combustion - fixed bed
Maren W. Kveinå	Norway	F	CO_2 emission reduction by CO to carbon / CNF - Fixed bed
Yun Liu	South Korea	F	Low temperature CO_2 capture / TGA
Jithin Gopakumar	India	M	Ethylene oxychlorination on Cu based catalysts
Hammad Farooq	Pakistan	M	Carbon formation and catalysis in the conversion of methyl chloride and silicon into dimethyldichlorosilane
Jørgen L. Grinna	Norway	M	Low temperature CO_2 capture by solid sorbents
Vilde Vinnes Jacobsen	Norway	F	Production of olefins from waste plastics
Susanne K. Stokkevåg	Norway	F	Oxidation of methanol to formaldehyde (MTF) over Ag catalysts
Anne Charlotte G. Wold	Norway	F	Kinetic study of processes for high temperature CO_2 capture by solid sorbents
Jon Arve Selnes	Norway	M	Catalytic methane abatement for natural gas engines
Eirik Søreide Hansen	Norway	M	Hydrogen production from biomass derived compounds by sorption enhanced reforming
Julie Christine Claussen	Norway	F	Polymers Assisted Preparation of Iron based Fischer-Tropsch Catalysts for biomass to fuel



Communication and Dissemination 2019

iCSI Plenaries

Olsbye, Unni: Selective partial oxidation of methane - the chemical looping approach. Robert Karl Graselli Foundation Irsee VIII Symposium; 2019-05-23 - 2019-05-26

Olsbye, Unni: Zeolite catalysis - what can we learn from Temporal Analysis of Products (TAP) experiments? Zeolites, Prospects & Challenges 7th edition; 2019-05-27 - 2019-05-29

Olsbye, Unni: Natural Gas Conversion in Microporous Catalysts, Zeotypes and Metal Organic Frameworks. 2019 Award for Excellence in Natural Gas Conversion 12th Natural Gas Conversion Symposium (NGCS); 2019-06-02 - 2019-06-06, San Antonio, Texas

Olsbye, Unni: Catalytic conversion of gas phase molecules over UiO-67 Zr-MOFs - Two case studies. Beilstein Nanoporous Symposium 2019; 2019-11-12 - 2019-11-14

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

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

iCSI Keynote lectures

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

Fjellvåg, Asbjørn Slagtern; Waller, David; Skjelstad, Johan; Sjåstad, Anja Olafsen: Ni-loss and Grain Reconstruction of Pd/Ni alloys. Defect-Chemical Nature of Advanced Energy Materials; 2019-10-19 - 2019-10-22, Tromsø, Norway

iCSI associated invited lectures

Svelle, Stian: Direct conversion of methane (to methanol): Is it feasible? Innovative catalysis and sustainability - Scientific and Socio-Economic Aspects, Winterschool; 2019-01-07 - 2019-01-11,

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

Hval, Halvor Høen; Tripathi, Alok Mani; Fjellvåg, Helmer: High Energy Density Electrodes for Lithium-ion Batteries and Operando Studies. MoZEES Annual Meeting; 2019-04-24 - 2019-04-25,Son, Norway

Hval, Halvor Høen; Tripathi, Alok Mani; Ruud, Amund; Emerich, Hermann; Forseth, Sissel; Nilsen, Ola; Fjellvåg, Helmer: Make Batteries Safe Again. Energiforskningskonferansen 2019; 2019-05-21 - 2019-05-21, Oslo, Norway

iCSI Publications and conference contributions 2019

IIA1: 21st Century Ammonia Oxidation and Nitric Acid Technology Development

Journal Publications

Bundli, Silje; Dhak, Prasanta; Jensen, Martin; Gunnæs, Anette Eleonora; Nguyen, Phuong Dan; Fjellvåg, Helmer; Sjåstad, Anja Olafsen: Controlled alloying of Pt-Rh nanoparticles by the polyol approach. Journal of Alloys and Compounds 2019; Volume 779. s. 879-885

Fjellvåg, Asbjørn Slagtern; Waller, David; Skjelstad, Johan; Sjåstad, Anja Olafsen: Grain Reconstruction of Pd and Pd/Ni Alloys for Platinum Catchment. Johnson Matthey Technology Review 2019; Volume 63.(4) s. 236-246

Kumar, Susmit; Waller, David; Fjellvåg, Helmer; Sjåstad, Anja Olafsen: Development of custom-made bimetallic alloy model systems based on platinum-rhodium for heterogeneous catalysis. Journal of Alloys and Compounds 2019; Volume 786. s. 1021-1029

Salman Ata ul Rauf; Hyrve, SM; Regli, Samuel K.; Zubair, Muhammad; Enger, Bjørn Christian; Lødeng, Rune; Waller, David; Rønning, Magnus;: Catalytic Oxidation of NO over LaCo1-xBxO3 (B = Mn, Ni) Perovskites for Nitric Acid Production, Catalysts. 2019, 9:429.

Oral Presentations

Rønning, Magnus; Salman, Ata ul Rauf; Regli, Samuel K.; Enger, Bjørn Christian; Lødeng, Rune; Waller, David;: Revealing the Structural and Chemical State of Platinum Nanoparticles during Oxidation of NO to NO_2 at Nitric Acid Plant Conditions. NAM26, 2019 North American Catalysis Society Meeting; 2019-06-23 - 2019-06-28, Chicago, Illinois

Fjellvåg, Asbjørn Slagtern; Waller, David; Skjelstad, Johan; Sjåstad, Anja Olafsen: Ni-loss and Grain Reconstruction of Pd/Ni alloys. Defect-Chemical Nature of Advanced Energy Materials; 2019-10-19 - 2019-10-22, Sommarøy, Norge

IIA3: Frontier Formalin Technology Development

Journal Publications

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

Oral Presentations

Lervold, Stine; Arnesen, Kamilla; Beck, Nikolas; Lødeng, Rune; Yang, Jia; Bingen, Kristin; Skjelstad, Johan; Venvik, Hilde Johnsen. Morphology and activity of electrolytic silver catalyst - For reactions relevant to partial oxidation of methanol to formaldehyde (MTF). EuropaCat 2019 14th European Congress on Catalysis; 2019-08-18 - 2019-08-23, Aachen, Germany

IIA4: PVC Value Chain: World Class Energy and Raw Material Efficiency for the Production of Chlorine and Vinyl Chloride Monomer (VCM)

Journal Publications

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

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

Oral Presentations

Kumar Rout, Terje Fuglerud, Marco Piccinini, Endre Fenes, Hongfei Ma, De Chen: Combined Solid- and Gas Phase Kinetic Modelling: Ethylene Oxychlorination over K-Promoted Cu/Al_2O_3 Catalyst, The 12th Natural Gas Conversion Symposium; 2019-06-02 - 2019-06-06, San Antonio, Texas

Hongfei Ma, Kumar Rout, Terje Fuglerud, Marco Piccinini, Endre Fenes, De Chen: Co-Promoting Effects of Mg and K in Ethylene Oxychlorination, The 12th Natural Gas Conversion Symposium; 2019-06-02 - 2019-06-06, San Antonio, Texas

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

Kumar Rout, Terje Fuglerud, Marco Piccinini, Endre Fenes, Hongfei Ma, De Chen: El Impregnated Mesoporous Carbon Spheres As Ideal Sorbent for Post-Combustion CO_2 Capture from Natural Gas Power Plant, The 12th Natural Gas Conversion Symposium; 2019-06-02 - 2019-06-06, San Antonio, Texas

Liland, Shirley Elisabeth Sjø; Rout, Kumar Ranjan; Yang, Jia; Chen, De: Operando Study of Surface Oxygen Coverage and Redox Reactions on Ni-Co Catalyst during Methane Combustion. NAM26, 2019 North American Catalysis Society Meeting; 2019-06-23 - 2019-06-28, Chicago, Illinois

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

Selleri, Tommaso; Hu, Wenshuo; Gramigni, Federica; Fenes, Endre; Rout, Kumar Ranjan; Nova, Isabella; Tronconi, Enrico; Gao, Xiang; Chen, De; Cen, Kefa: A HONO-Based Mechanism for the Reduction Half-Cycle in the Low Temperature SCR of NO over Cu-SSZ-13. NAM26, 2019 North American Catalysis Society Meeting; 2019-06-23 - 2019-06-28, Chicago, Illinois

Ma, Hongfei; Fenes, Endre; Qi, Yanying; Wang, Yalan; Rout, Kumar Ranjan; Fuglerud, Terje; Chen, De: Kinetic Analysis and Design of Catalytic Redox Cycles in Ethylene Oxychlorination. EuropaCat 2019 14th European Congress on Catalysis; 2019-08-18 - 2019-08-23, Aachen, Germany

iCSI Poster Presentations

Wang, Yalan; Xiao, Ling; Qi, Yanying; Zhu, Yi-An; Yang, Jia; Chen, De; Holmen, Anders: Microkinetic model aided rational catalyst design for light olefins production from synthesis gas through hybrid semi-empirical approach. 2019 North American Catalysis Society Meeting; 2019-06-23 - 2019-06-28, Chicago, Illinois

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

Qi, Yanying; Fenes, Endre; Ma, Hongfei; Wang, Yalan; Rout, Kumar Ranjan; Fuglerud, Terje; Chen, De: Insights into potassium promoter effects on $CuCl_2/\gamma\text{-}Al_2O_3$ catalyzed ethylene oxychlorination. EuropaCat 2019 14th European Congress on Catalysis; 2019-08-18 - 2019-08-23, Aachen, Germany

IIA 5: The Next Step in Direct Activation of Lower Alkanes

Journal Publications

Brogaard, Rasmus Yding; Kømurcu, Mustafa; Dyballa, Michael Martin; Botan, Alexandru; Van Speybroeck, Veronique; Olsbye, Unni; De Wispelaere, Kristof., Ethene Dimerization on Zeolite-Hosted Ni Ions: Reversible Mobilization of the Active Site. ACS Catalysis 2019 ;Volume 9.(6) s. 5645-5650

Dyballa, Michael Martin; Pappas, Dimitrios; Kvande, Karoline; Borfecchia, Elisa; Arstad, Bjørnar; Beato, Pablo; Olsbye, Unni; Svelle, Stian: On how copper mordenite properties govern the framework stability and activity in the methane-to-methanol conversion. ACS Catalysis 2019; Volume 9.(1) s. 365-375

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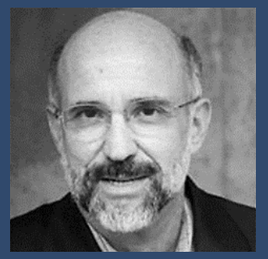

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