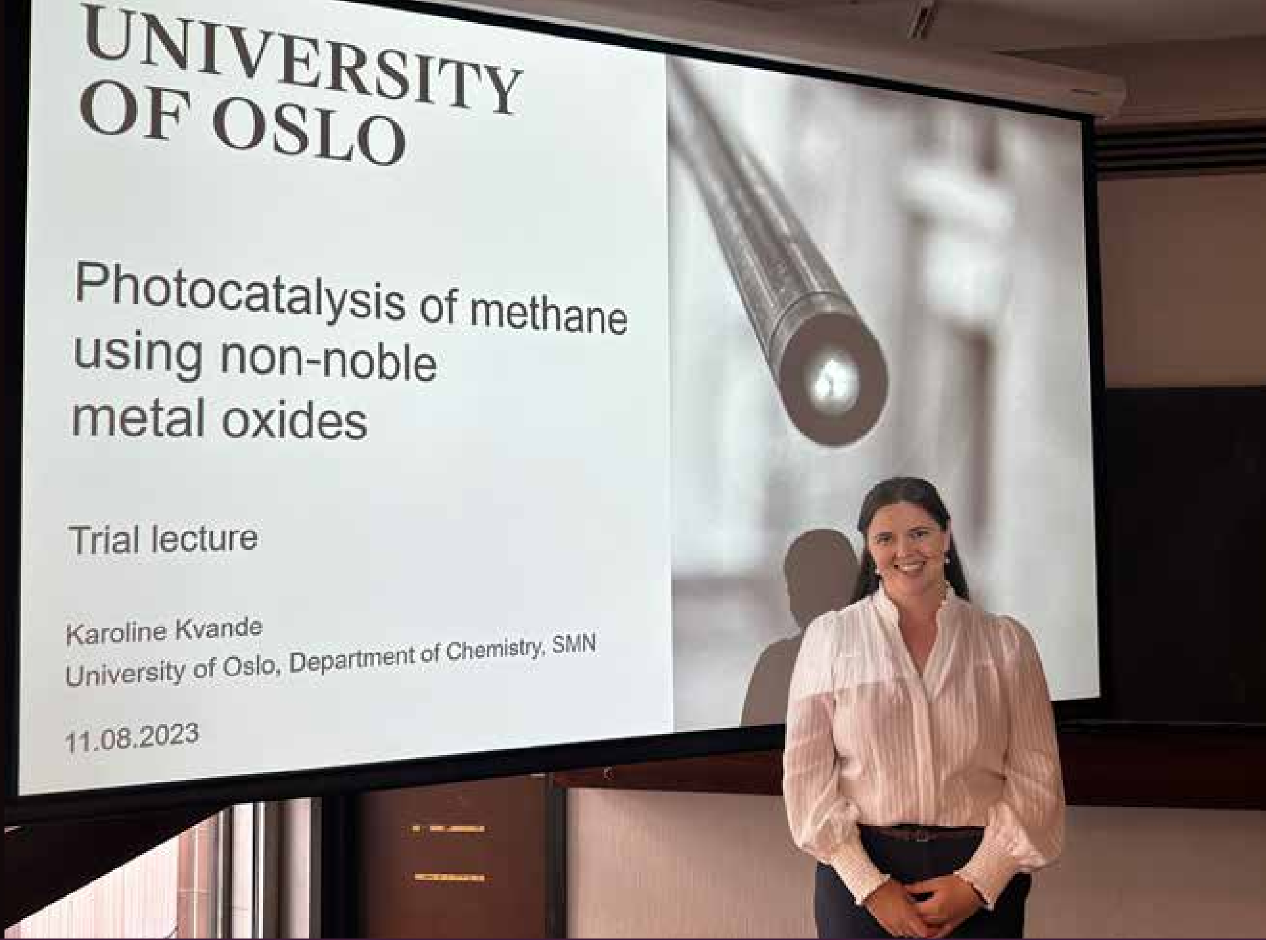


iCSI

industrial Catalysis Science and Innovation

Annual Report 2023

Norwegian Centre for Research-based Innovation

NTNU

iCSI Partners

Norwegian Centre for Research-based Innovation

NTNU   SINTEF   UiO University of Oslo

YARA   TOPSOE   INEOS Inovyn

K·A·Rasmussen NORWAY   dynea®

Funded by The Research Council of Norway

Cover photo: PhD candidate Karoline Kvande at the defense of her PhD thesis August 11, 2023. Photo: Private

2023 Summary

It is with a certain sadness, but also with pride that we sum up 2023, which was the year the SFI *industrial Catalysis Science and Innovation* (iCSI) was completed. We have achieved a lot in these eight years, and the most important results and their significance will be discussed in more detail in the final report from the centre. However, it is now time to see what we have achieved this past year.

Science has progressed in all Industrial Innovation Areas, and on page 16 to 19 we present two of this year's highlights. Karoline Kvande has shown how both international and cross-disciplinary collaboration within iCSI adds value to the research. Jithin Gopakumar has been in Grenoble using the Swiss-Norwegian Beamline for X-ray spectroscopy experiments, which unravelled the transformations of ruthenium catalysts during nitric acid production.

Nineteen reviewed papers were submitted and accepted for publishing in 2023 and so far in 2024. The publications were from IIA1, IIA4, IIA5 and IIA6, and ten of them were published with international collaboration partners, while industry partners were co-authors for twelve of the publications. Even though iCSI is shutting down, more papers from the research are in the pipeline to be published in the coming year(s). One of the aims for iCSI when starting up was to produce 100 scientific papers, and the finish line for that was just reached at the time of writing this summary.

iCSI was represented at several international conferences in 2023, and the most important this year was EuropaCat 2023 in Prague. More than 30 Norwegian catalysis researchers were present there and many of them showed iCSI research results, both orally and on posters. At the closing session of the congress, Centre Director Hilde Johnsen Venvik, co-ordinator Anne Hoff and professor Magnus Rønning from iCSI went on stage to invite the European catalysis community to EuropaCat 2025 in Trondheim. It is with joy and excitement that we look forward to, together with our Nordic colleagues, welcoming everyone to the Clarion Hotel and Pirsenteret next year.

A complete list of publications and conference contributions from iCSI and associated researchers in 2023 can be found on pages 58-65.

This year, the CATHEX project, supporting collaboration with international partners, funded a three-month sabbatical stay at the University of Cape Town, South Africa for iCSI professor Anja Sjåstad and a one-month stay for iCSI associated postdoc Felix Herold, NTNU, at the same place. In addition, several of the professors and young researchers from the collaborating universities came to Trondheim to participate in the joint iCSI/CATHEX seminar in June. This event gathered as many as 70 catalysis researchers to a four-day "catalysis festival", where two days were spent summing up results from the eight years of iCSI.

Educating master's students is important to iCSI. In 2023, ten graduating master's students were associated with iCSI, four of whom delivered directly into the ongoing projects. The gender balance within iCSI is maintained, with all personnel categories close to a 40/60 distribution.

Two candidates, Karoline Kvande (UiO) and Wei Zhang (NTNU), finalised their PhD theses with defences in August and November, respectively. iCSI congratulates them and their supervisors, Professor Stian Svelle and Professor De Chen!

PhD candidate Youri van Valen finished his industrial exchange in March with a one-month stay at K.A. Rasmussen. He was the last of a total of nine candidates who have had the opportunity to partake in a two-month exchange in order to experience everyday industrial life and contribute to the hosts' problem-solving with up-to-date knowledge. iCSI is grateful to have had industrial partners who see the value of this and opened their doors for exchange of personnel and knowledge.

The representation on the iCSI Board has changed for one of the industry partners in 2023, with Ann Kristin Lagmannsveen taking over from Thomas By as K. A. Rasmussen's board representative in March. We thank everyone on the board, as well as all the scientists for their efforts for iCSI throughout this and all the previous years!

Content

From the iCSI/CATHEX seminar June 2023.

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 and industrial competitiveness, as well as future chemical processing and energy conversion with the smallest possible environmental footprint. The industrial partners involved supply key sectors of the global market (e.g. catalysts, chemicals, fertilizer, plastics, fuels), 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 enables 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 into 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: Thor Nielsen

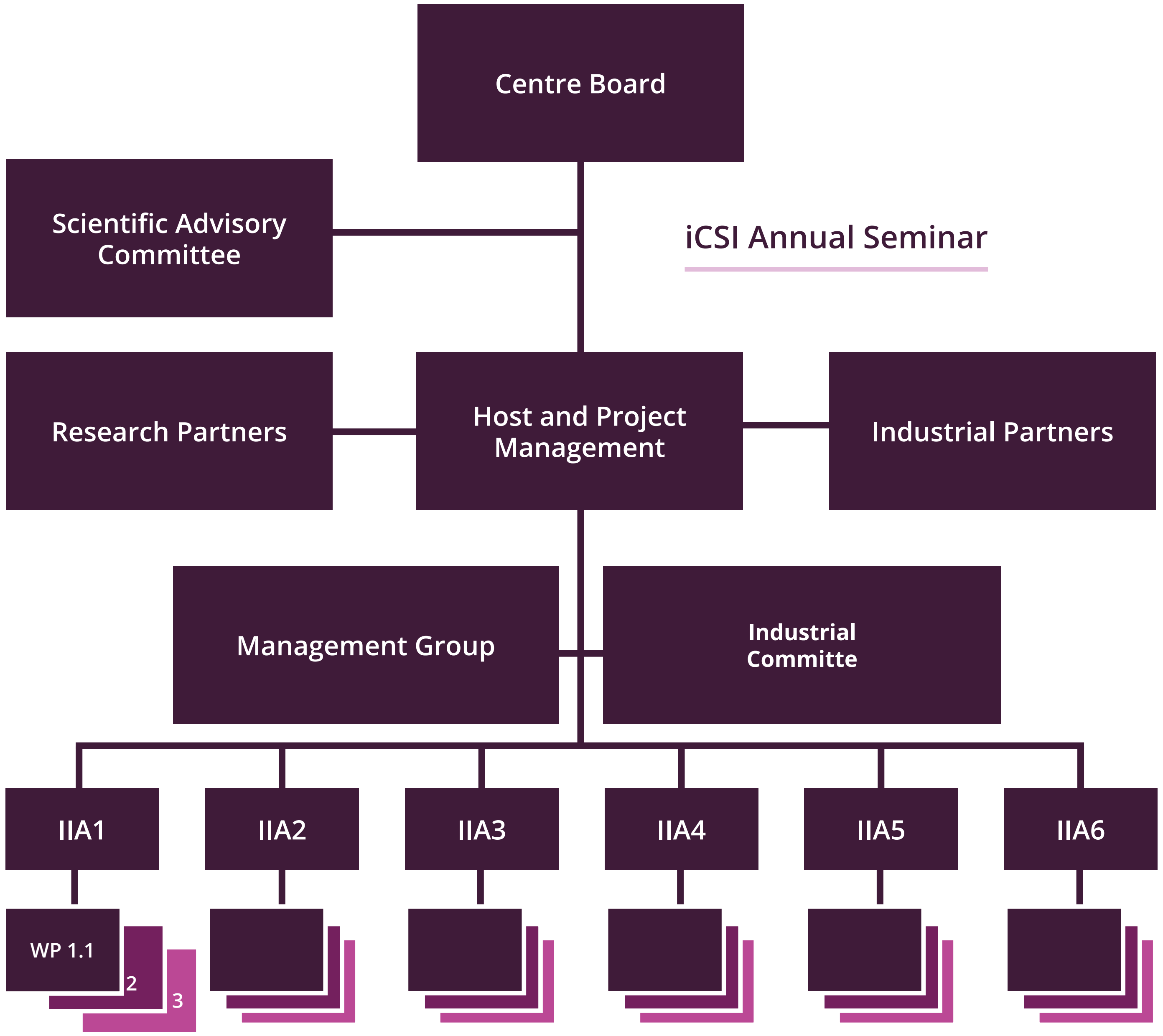
iCSI's main objective is to boost industrial innovation and competitiveness and provide efficient, low-emission processes.

This aim can be achieved through:

- *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) serves as the 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, INEOS Inovynand 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 (IIA1-5) 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 the 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.

INEOS Inovyn

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

YARA

Yara International ASA is a Norwegian-based chemical company with fertilizer as its largest business area. Yara also works with chemical and environmental solutions for industrial plants, vehicles and marine vessels. In addition to being present in more than 60 countries, Yara operates two industrial sites in Norway, Porsgrunn and Glomfjord, with approx. 700 employees. In iCSI, Yara aims to further strengthen its global competitiveness through innovation.

TOPSOE

Topsoe is a catalyst producer and process plant technology developer based in Denmark. Topsoe wants to be the global leader within carbon emission reduction technologies for the chemical and refining industries. By perfecting chemistry for a better world, we enable our customers to succeed in the transition towards renewable energy.

K·A·Rasmussen NORWAY

K.A. 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. K.A. Rasmussen has specialized in technology for producing structured catalysts for the Ostwald process and silver particles for the oxidation of methanol. In iCSI, K.A. 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.

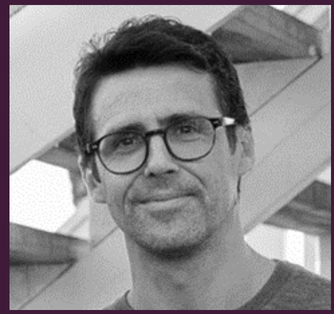
dynea®

Dynea As is a Norwegian-owned specialty chemical company for sustainable wood adhesives, industrial coatings, specialty adhesives & polymers and surfacing solutions, with production sites in Norway, Denmark and Hungary, and licensing of the wellknown Dynea Silver Catalyzed Formaldehyde technology, fasil®. In iCSI, Dynea aims to continue its technological leadership in formalin production for improved plant operations and reduced cost for its fasil® technology.

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.

Pablo Beato from Haldor Topsøe continued as Chair of the Board in 2023. In March 2023, Ann Kristin Lagmannsveen replaced Thomas Bye as K.A. Rasmussen's representative.



Dr. Pablo Beato

Lead Scientist directing the Atomic-Scale Analysis Department at Haldor Topsøe

Lars Axelsen

General Manager of Technology Sales & Licensing at Dynea.

Torgeir Lunde

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

Ann Kristin Lagmannsveen

Research and Development engineer at K.A. Rasmussen

Tigran Margossian

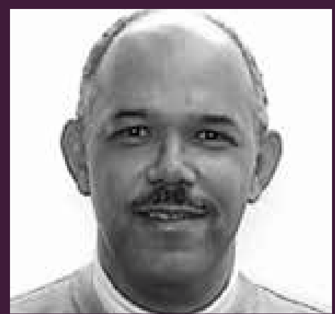
Research and Development Manager at INEOS Inovyn

Professor Einar Uggerud

Head of Department of Chemistry at the University of Oslo

Professor Karina Mathisen

Vice Dean for Education and Dissemination at NTNU's Faculty of Natural Sciences



Dr. Duncan Akporiaye

Research Director at SINTEF Industry.

Dr. Aase Marie Hundere

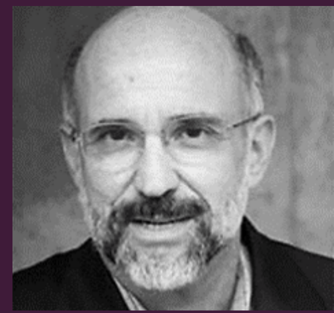
Special advisor RCN, with Responsibility for Nanotechnology and Advanced Materials

Scientific Advisory Committee

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.

Professor Alessandra Beretta

Politecnico di Milano, Italy



Professor Enrique Iglesia

University of California, Berkeley, USA

Professor Graham Hutchings

Cardiff University, United Kingdom

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 (50 % position) and an Economy Advisor (20 % position).

Hilde J. Venvik

Professor
iCSI Centre Director

Anne Hoff

Senior advisor
iCSI Coordinator

Hilde M. Flaathe

Financial Project Advisor
iCSI Economy advisor

Researcher Portrait: Hilde Johnsen Venvik

As the last in the series of portraits of professors in the iCSI family, Centre Director Hilde Johnsen Venvik will this year tell a little about herself and her motivation for carrying out catalysis research.

Hilde was born in Bergen and raised in Tromsø, and is proud of coming from above the Arctic Circle. She loves the nature up there, so much that she invited the world's academic gas conversion community to a conference in Tromsø in 2016. There, she and her mother guided 30 of the participants on a post-conference hike in the mountains. Not all participants were prepared for low temperatures, but Hilde's mother had home-knitted hats and mittens for everyone, so it ended well. In many ways, this story illustrates Hilde's qualities.

Her path to catalysis went through a master's degree in solid state physics and experimental characterisation, and she proceeded with a PhD in surface science with catalytic model systems. In the late nineties, the catalysis group at NTNU was dominated by chemical engineers, and as a physicist she brought with her some new perspectives. These included a better understanding of basic material and surface properties (quantum mechanics, crystal structure, surfaces), of measurement techniques such as spectroscopy and microscopy based on photons and electrons, signal processing and statistics – as well as a good understanding of transport phenomena and crystal growth.

"We were completely at the forefront of research when the STM instrument came to NTNU in 1991, and I got the first student project on this instrument!"

When asked about the main difference between physicists and chemical engineers, she says: "Physicists are perhaps more openly investigative and concerned with the laws of nature, while chemical engineers are most concerned with meaningful problem solving and how to find environmentally friendly solutions to the world's challenges". Hilde wants to take the best from the two worlds.

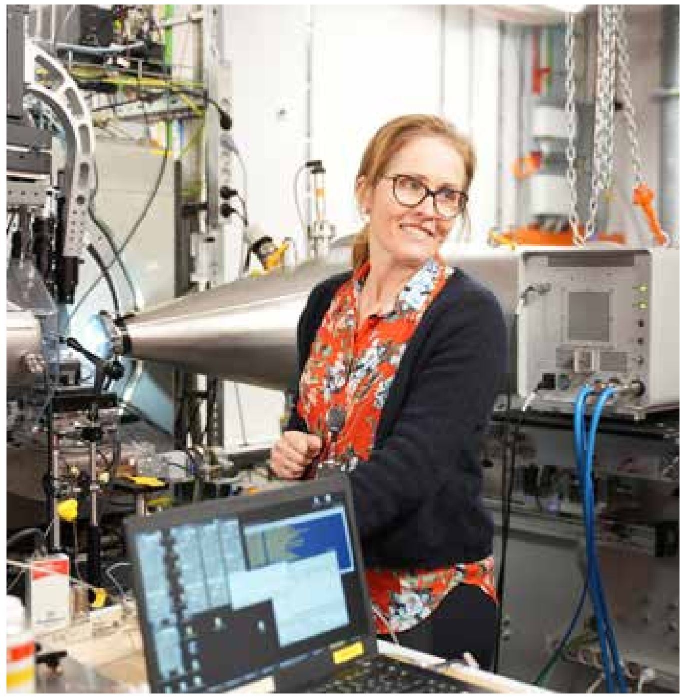
Many people have helped her on her way, and the two most important are without doubt her PhD supervisor Professor Anne Borg with her clear thought and thoroughness in experimental work, together with Professor Anders Holmen with his international ambitions and skills as a builder of research groups.

For Hilde, growing up in Tromsø was characterised by safety and freedom, where she was allowed to take responsibility for her own activities. There was a lot of horse riding and volleyball in her teenage years, and these were arenas that developed her skills and mastery. As an adult, she believes that it is important for young people to be concerned with something outside of oneself.

Hilde has continued to take responsibility for the community. She now holds several professional positions of trust, both nationally and internationally. She is Chair of the Catalysis group in the Norwegian Chemical Society and is Vice President of the European catalysis federation, EFCATS. **"If the tasks are important (for the Norwegian community or NTNU), then someone has to do it. It is an international *dugnad** that gives something back in the form of networking."**

Teaching is an important part of Hilde's tasks as a professor, and she thinks most of today's students are incredibly fine people. "At NTNU, we are privileged to work with so many great young people - professionally skilled, committed to society and the environment, caring for each other. I sincerely believe that they help keep my own mind and body a little younger. And maybe I'm not 100% objective, but I think Trondheim has the world's best student community, created through student volunteerism".

** Norwegian expression for voluntary work for the common good*



Hilde Venvik was for a three-year period appointed as a Lise Meitner-professor at the Department of Chemical Engineering at Lund University. These professorships are granted to leading researchers of the underrepresented gender who are nominated to work at the faculty as a visiting professor and act as a role model for younger researchers, teachers and students. Photo from the MAX IV synchrotron at Lund University.

Hilde with international colleagues in EFCATS Council, Prague 2023.

There are two messages she repeats to all students:

- **You must carefully consider how catalyst activity is defined and measured**
- **You have to think through what a measurement actually means (what is perturbation and response and what can be interpreted - and NOT interpreted - out of it).**

What is your opinion on the status of Norwegian catalysis research compared to what is happening internationally?
"Given the resources we have, I think we can be proud of ourselves! But we still struggle to achieve the levels that our top notch European and American colleagues reach. The SFIs inGAP and iCSI have been key in this respect, and also provided us with distinct profiles that are recognised abroad. But even if they resource-wise (human and funding) are "leading" in a Norwegian context, it is far from the levels available in the best European labs. What we experience, is that 3 years for an experimental PhD often is too short to go into the depth of a topic. We need long term projects with several generations of PhD candidates studying a topic."

iCSI is now shutting down as a centre after eight years. What has been the most fun while leading it?

"It has been the interaction with and appreciation from the inspirational competent industrial partners, the collaborative spirit existing between the research groups, and seeing the PhD candidates develop and complete their research.

At iCSI, we have achieved almost everything I hoped for when we started in 2015 - in education, publishing and research. The resulting innovations are more difficult to document or predict, but we have contributed a lot of new knowledge that the industry will make use of in various ways, in addition to a small number of patenting initiatives. We could possibly have been better at popularising our results, but we have had individuals who have demonstrated both the will and good ability to do this." Hilde also insists on adding that SFI is a unique instrument for innovation-driven research in a national and international context. She believes that history will show that it has been more important than what we see and are able to document today.

Artificial intelligence (AI) is predicted to change our world in dramatic ways. What possibilities does Hilde envision with this tool - for better or for worse? "The possibility of insight (science) and profit (business) is enormous if you are able to use it to connect data, physical properties and theoretical models. This involves quite extreme system-

The northern Norwegian nature has given Hilde and her family many good experiences. Left: Skiing on Kjølen, Kvaløya. On the right, Hilde and Ola together with their sons Øystein and Gaute at the top of the mountain Hamperokken (1404 m above sea level)

atisation and curation work, but if I were in a company, I would not hesitate to start now on the materials and chemical processes that are critical to my profitability. But good experiments will never go out of style – only how to interpret and use them. Hopefully there will be AI resources to help solve the environmental and climate problems."

AI also represents a challenge in terms of how we test and evaluate students, but that can be solved. We also did a lot of sensible things the old way, offline with "pen and paper".

Work isn't the only part of the professor's life. When she feels good at home, it is often an inspiration to perform well at work. Life is at its best when she is with her newborn grandson, on a mountaintop in glorious weather, after a long day in the garden - or when doctoral and master's students achieve their goals, when students report that they find her teaching meaningful or when a manuscript they have been working hard on for a long time is published.

Other things that inspire Hilde can be: People with commitment (whether for science or the community in other ways), knowledge (almost in any field), practically all kind of challenges (though not too abstract problems), and music, art and literature. She claims that research must be driven by an inner curiosity about nature and people and a desire to make the world better, not by a desire for prestige, status and wealth - although recognition is always nice.

Hilde and her husband Ola have raised three children in parallel with their careers, and she is very proud of them all and appreciates that they have grown up to become independent, decent people who are able to make good choices in their lives. But she is also proud of all her doctoral students and that she in her career has to some extent managed to follow her own ideas and concepts, and from there conducted solid research.

Finally, Hilde, what are you looking forward to now that iCSI will soon be a closed chapter?
"In a not-too-distant future, I will take a research term/sabbatical. Then I will take a look at what kind of research I find most meaningful to devote time to. But before that, I look forward to, together with Anne Hoff and others, bringing together the entire European catalysis society in Trondheim for EuropaCat 2025! Another project, HYDROGENi, is already running with me on board. I will also teach more, especially chemical reaction engineering. **You know, there are tremendous problems out there that we need chemical engineers to help solve."**

In 1994, it was not common for women with children inside or outside of their belly to get doctorates. Adresseavisen 1994

Blivende mamma og dr.ing.

SVEIN INGE MELAND

Dr.ing-student Hilde Venvik (26) har to «babyer» underveis; doktoravhandlingen om katalyse som skal være ferdig i 1997, og en liten en i magen som har meldt ankomst i mars. Hildes forklaring på doktorkøen ved NTH er bra oppfølging og bedre finansieringsmuligheter enn ellers i universitetsverden.

Hilde Venvik syntes hun var så godt i gang da hun holdt på med diplomoppgaven på NTH at hun valgte å ta tre-fire år ekstra for å bli dr. ing. Jenta fra Tromsø er ikke i tvil om at doktorgrader blir bare viktigere og viktigere for at norsk industri skal få god nok kompetanse til å hevde seg i konkurransen med andre land.

– Industrien vil forandre seg og kompetansenivået heves. Dette skjer i hele Europa, sier Hilde. Selv kan hun tenke seg å reise utenlands og studere videre etter at hun er ferdig med avhandlingen.

NTHs store fordel er kontakten med næringslivet og mulighetene til å finansiere studiene for doktorkandidatene. Hilde får penger fra Statoil via Vitenskapsakademiet i Oslo. Vanlig stipendiatlønn er 206 000 kroner i året. Nå er det slett ikke alle som begynner med avhandlingen som blir ferdig og kan pryde seg med dr.-tittel. Hilde tror det avhenger av hvor godt fagmiljøene rundt studenten virker.

– De fleste trenger hjelp for å komme seg videre når de «møter veggen». Jeg har inntrykk av at det varierer sterkt fra fagmiljø til fagmiljø hvor god støtte man får. Selv er jeg godt fornøyd.

Dr.ing.-studenten er pålagt å undervise en del ved siden

KOMMENDE DOCTOR: *Hilde Venvik er en av mange NTH-studenter som går videre og tar doktorgraden.* Foto: STEIN FJESME

Welcome to Trondheim and EuropaCat 2025!

The European Congress on Catalysis (EuropaCat) takes place biennially and has been the largest and most important catalysis conference in Europe since 1993. It is organised under the auspices of the European Federation of Catalysis Societies (EFCATS; a non-profit AISBL), and the local organiser is appointed following an application to the EFCATS Council, which consists of representatives from each of the national societies. EuropaCat 2023 took place in Prague during the last week of August, and the catalysis communities in the Czech Republic, Hungary, Poland and Slovakia jointly organised this event.

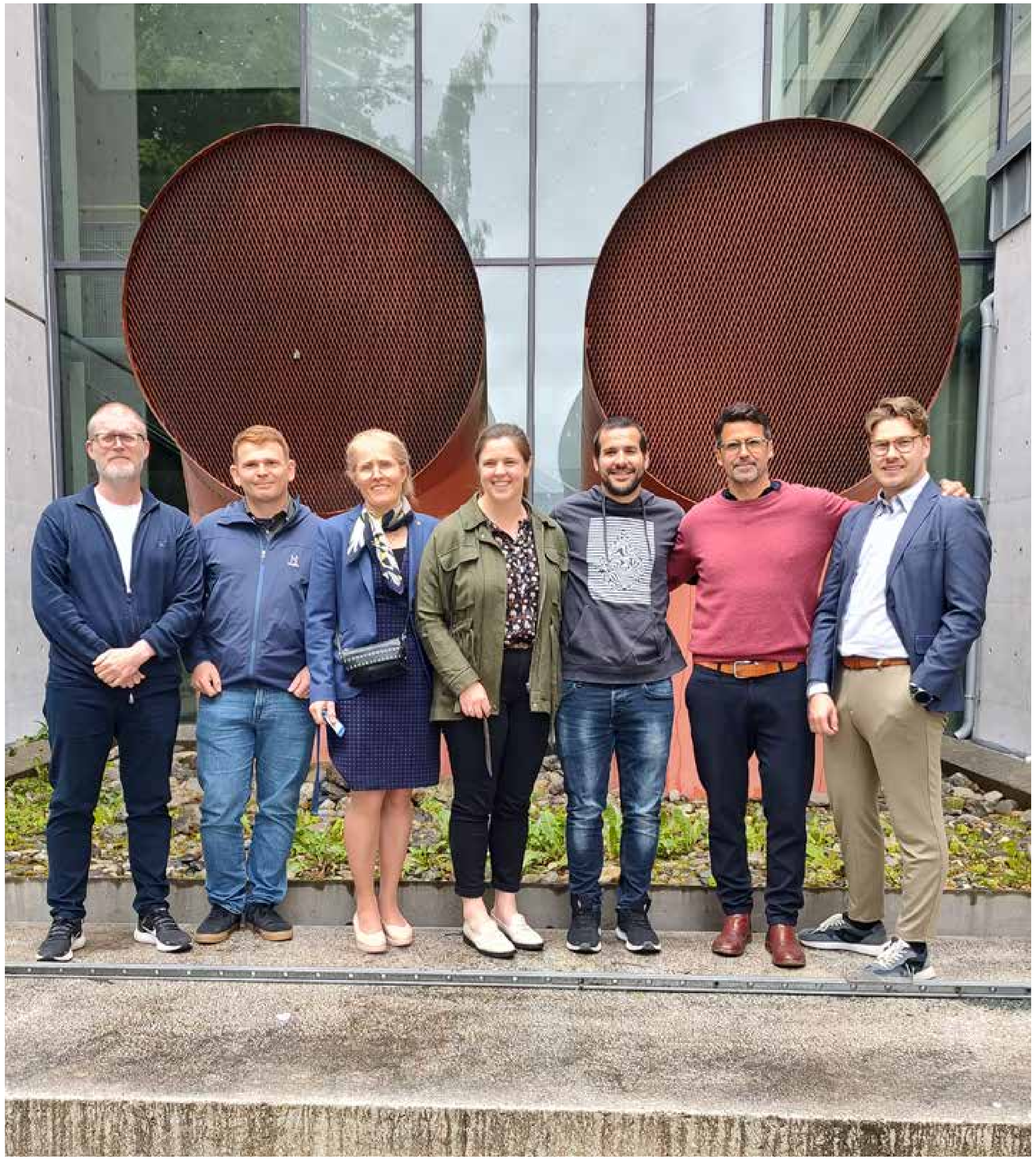
It is with pride and excitement that we invite the European catalysis community to EuropaCat 2025 in Trondheim. This will be the 16th European Congress on Catalysis under EFCATS and organised as a joint effort of the Nordic Catalysis Societies.

Between 1000 and 1500 participants are expected, with the largest group from academia (from senior faculty to PhD students) but also significant attendance from catalyst suppliers, the process industry, and their subcontractors. For all these different groups, we aim to create a vibrant catalysis hub at Clarion Hotel Trondheim and Pirsenteret on the waterfront.

Hilde Johnsen Venvik acts as Chair of the conference, while Anne Hoff and Magnus Rønning are Vice Chairs. They urge all with interests in catalysis to join and bring along excellent science, hard work, bright ideas, successful catalyst development, innovative solutions and an open mind. It is clear that mastering "the force" of catalysis will be of utmost importance to the resources and environmental challenges that lie ahead for humanity.

Hilde Johnsen Venvik on stage during the last day of EuropaCat 2023 in Prague, inviting the European catalysis community to EuropaCat 2025 in Trondheim.

Scientific Highlights 2023:
Collaboration is the path to success



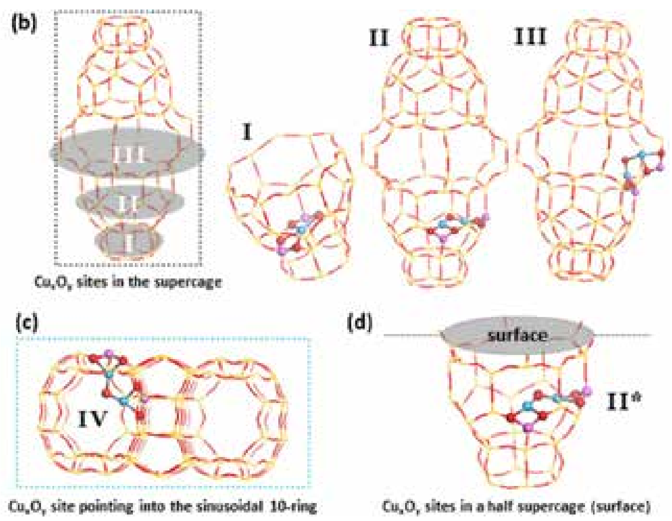
Good science makes good friends. From left to right: Stian Svelle (IIA5 leader), Dimitrios Pappas (iCSI PhD candidate); Hilde Venvik (iCSI Centre Director); Karoline Kvande (iCSI PhD candidate); Izar Capel Berdiell (iCSI Postdoc); Pablo Beato (senior scientist at Haldor Topsøe A/S); Bjørn Gading Solemsli (iCSI PhD candidate)

Within IIA5, collaborations have been the driving force from the get-go of iCSI. The core of that has been the association between our group in Oslo, Pablo Beato at Topsoe A/S in Copenhagen, and our friends and colleagues at the University of Turin. This partnership has strengthened our group through the possibility of knowledge-sharing across different fields and techniques such as chemical engineering and catalytic testing, inorganic chemical synthesis, as well as spectroscopic analysis.

Back in 2019, at the start of Karoline Kvande's PhD project, we wanted to build on the knowledge of direct methane oxidation reactions that was already established in the group at that time. In a then-recent paper by van Bokhoven and co-workers (V. L. Sushkevich et al. Science, 2017, 356 , 523 —527), it was shown that temperature-programmed reactions with methane could be used to illustrate differences in the oxidation onset of methane over a set of Cu-zeolites pretreated in oxygen. This paper laid the foundation for a synchrotron application to MAX IV in Lund, where we wanted to study, in-situ, the changes in the Cu environment, geometry, and oxidation state when oxidized Cu-zeolites were exposed to a reducing agent, while at the same time capturing the reactor effluent. This was planned for the end of February 2020, but due to the onset of the Covid-19 pandemic, our spectroscopy experts from Italy were, at the time, denied entry into the facilities. Our Cu-zeolite systems are extremely sensitive to moisture, and afterward, we learned that there were minor traces of water in the spectra, unfortunately not captured by the remaining teams' less-trained eyes. Many days and nights at the synchrotron were sadly wasted. However, believing in the potential of the experiment, we threw in another synchrotron application, this time at the European Synchrotron Radiation Facility in Grenoble (the Swiss-Norwegian beamline, BM31). After some more delays due to Covid-19, we were finally able to repeat the experiment more than 1.5 years after our first trip to Lund. In the end, our experiment was extremely successful and led to our publication in Chemical Science (2023). This should truly be attributed to the long-term planning and preparation we were given the opportunity to do, the amazing efforts and combined knowledge of the team on-site, as well as the continuous collaboration and progression of other projects that led to new ideas, small changes, and extensions to our primary experiment plan.

In addition to having prosperous collaborations within IIA5, the iCSI umbrella also allowed for potential partnerships. In IIA6, Moses Mawanga and Professor Edd Anders Blekkan developed a method for measuring heats of adsorption over different surfaces (microcalorimetry). This led us to explore the effects of both NH_3 and CH_4 adsorption on MCM-22; a hitherto untested zeolite framework for the methane-to-methanol reaction. The microcalorimetry results provided insight into the complexity of the MCM-22 framework and combined with testing and additional spectroscopy, they helped explain the activity of MCM-22 (or lack thereof) in the reaction. Due to fruitful discussions between the groups, we were finally able to publish the results in Industrial & Engineering Chemistry Research.

Overall, we are very pleased to have had the opportunity to collaborate across institutions and are certain that this has led not only to increased research quality and understanding, but also invaluable cultural exchange, fun moments, and friends spread all over the continent.



Representation of likely CuxOy-site positions in the MCM-22 channels. (b) Three possible positions for Cu_xO_y-sites within the supercage: I shows a four-coordinated site situated in the double 6-ring, while II and III are situated at possible T-sites in the supercage cavity. (c) represents a likely position (IV) within the sinusoidal 10-ring, and (d) shows how the supercage is opened up, exposing Cu-sites (e.g., II) on the external surface of the material. (From Kvande et al., Ind. Eng. Chem. Res. 2023)*

Publications

Karoline Kvande, Beatrice Garetto, Gabriele Deplano, Matteo Signorile, Bjørn Gading Solemsli, Sebastian Prodinger, Unni Olsbye, Pablo Beato, Silvia Bordiga, Stian Svelle, and Elisa Borfecchia: Understanding C-H activation in light alkanes over Cu-MOR zeolites by coupling advanced spectroscopy and temperature-programmed reduction experiments, Chemical Science, 2023, 14, 9704-9723

Karoline Kvande, Moses Mawanga, Sebastian Prodinger, Bjørn Gading Solemsli, Jia Yang, Unni Olsbye, Pablo Beato, Edd Anders Blekkan, and Stian Svelle: Microcalorimetry on Cu-MCM-22 reveals structure-activity relationships for the methane-to-methanol reaction, Industrial Engineering Chemistry Research, 2023, 62 (28), 10939-10950

Scientific Highlights 2023:
iCSI benefits from the collaboration with the European Synchrotron (ERSF)

One of the main objectives in the drive towards more sustainable chemical processes is to intensify the processes themselves, thereby reducing their carbon footprint and increasing energy efficiency. One such example is the oxidation of nitric oxide, one of the main steps in the chemical process that produces industrial nitric acid. Nitric acid is a corrosive mineral acid mainly used to produce nitrate fertilisers, which dramatically improve agricultural output in modern agrarian systems.

Commercial nitric acid production uses the century-old Ostwald process, which consists of three important chemical steps: Catalytic oxidation of ammonia using a Pt-Rh gauze catalyst; followed by gas-phase oxidation of NO to NO_2 using a series of heat exchangers, and finally, NO_2 absorption in water to produce nitric acid. Catalysing the bulky homogeneous gas-phase oxidation of NO to NO_2 may lead to about a 15% intensification of the Ostwald process (C. Grande et al., Ind. Eng. Chem. Res. 57, 10180-10186 (2018)). Supported Ru catalysts show promising activity and stability at ambient and 4 bar(g) pressures at industrial nitric acid production conditions.

Experiments at the ESRF have helped to decipher the enigma behind the Ru catalyst's capacity to oxidise nitric oxide at industrially relevant conditions, thus paving the way to intensifying a large established industrial process (J. Gopakumar et al., Catal. Sci. Tech. 13, 2783-2793 (2023).). *In-situ* X-ray absorption spectroscopy (XAS) at the Ru K edge (22.1172 keV) was carried out at the Swiss-Norwegian beamline (SNBL) BM31.

Figure 1 illustrates the experimental setup: X-rays continuously irradiated the γ-Al_2O_3-supported Ru catalyst during NO oxidation. An X-ray absorption near-edge structure (XANES) spectrum was collected every 8-10 seconds, precisely recording the changes in the Ru in the catalyst sample at isothermal conditions. A mass spectrometer (MS) was used to analyse O_2 and NO_2 in the product process gas.

Multivariate curve resolution-alternating least squares (MCR-ALS) data analysis of the in-situ XANES data collected during the experiment revealed two distinct components of Ru (as presented in Figure 2a). Component A was completely reduced (representing Ru0 in the metallic state) and component B was 30% oxidised. By synchronising the XANES and MS data acquisition rate, subtle changes could be observed in the Ru during NO oxidation. Figures 2c and 2f display the synchronised MCR-ALS contribution plot and the MS signals of O_2 and NO_2 in a 20-minute time frame.

The oxidation state of a fraction of Ru in the catalyst oscillates between slightly oxidised and completely reduced. To understand the oscillating behaviour, extended X-ray absorption fine structure (EXAFS) spectroscopy and X-ray photo-electron spectroscopy (XPS) analyses of the two components were performed, and a clear surface oxidation was observed in component B (as presented in Figures 2d and 2e).

The results reveal the mechanism behind NO oxidation at industrial nitric acid production conditions over γ-Al_2O_3-supported Ru catalysts, and suggest a method to further tune the performance of the Ru catalysts at demanding reaction conditions. Furthermore, the study demonstrates that with careful experimental design and data analysis from complimentary techniques, a bulk technique such as X-ray absorption spectroscopy can also probe the surface of the sample. Overall, the work highlights the capacity of in-situ X-ray tools to bridge the gap between laboratory- and industrial-scale reactions.

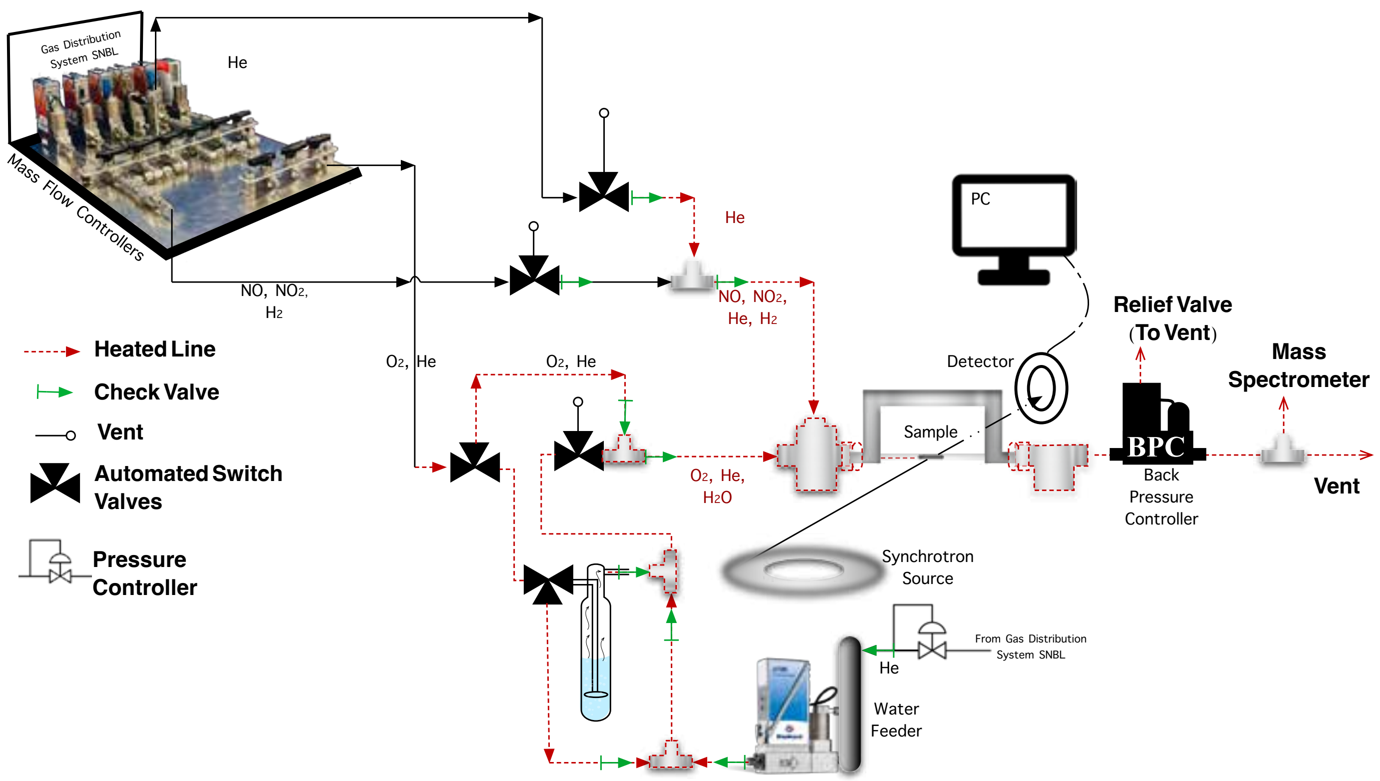


Figure 1 In-situ X-ray absorption experimental setup for oxidation of nitric oxide at beamline BM31.

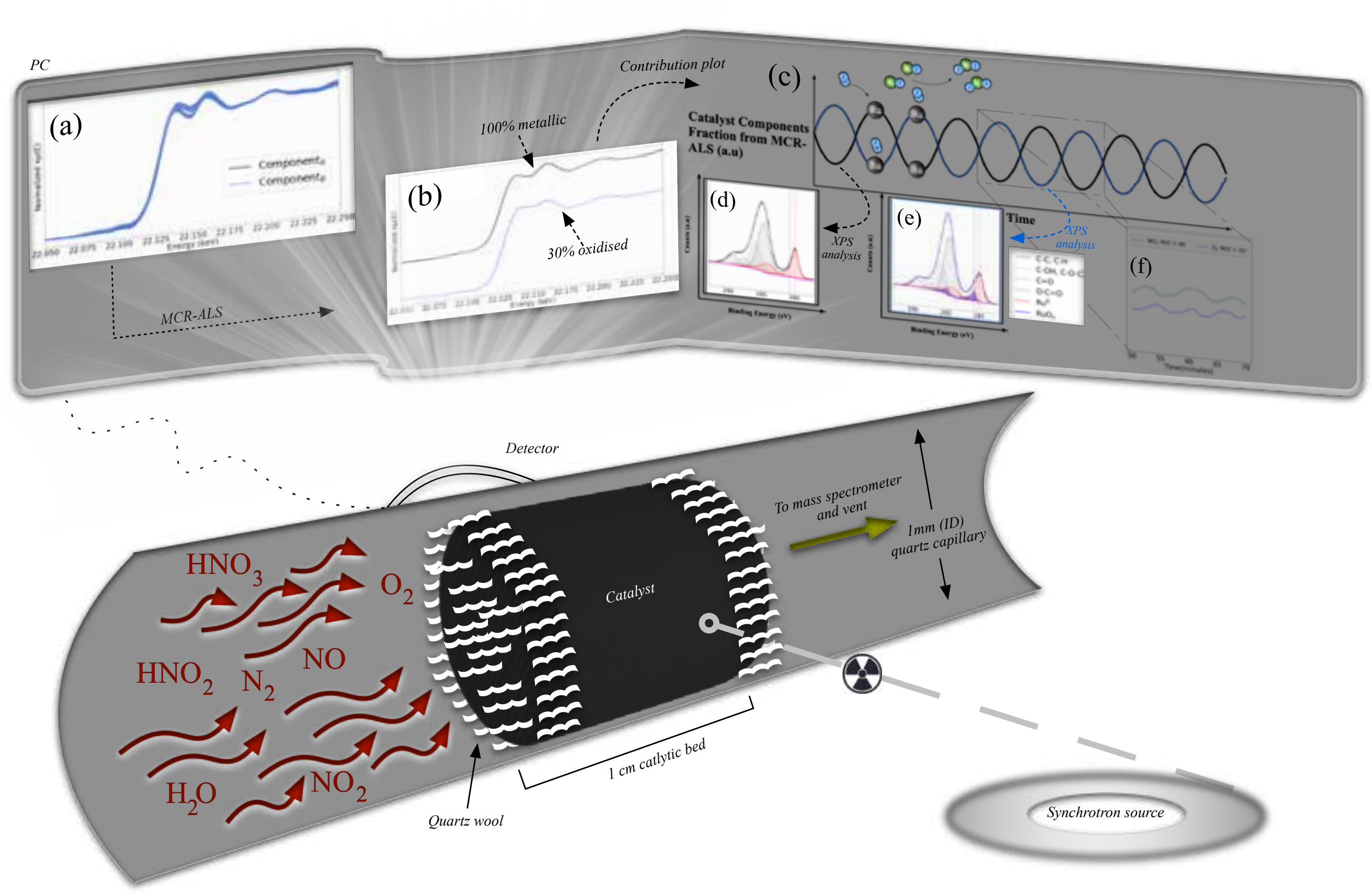


Figure 2 a) In-situ XANES profiles of γ-Al_2O_3-supported Ru catalysts collected during NO oxidation at 350°C. b) MCR-extracted components from the XANES data in (a). c) MCR-calculated contribution plot across 3 hours of XANES data collection. C 1s and Ru 3d XPS spectra of (d) component A and (e) component B. f) Collected mass spectrometer signal for O_2 and NO_2 during 20 minutes of a total of 3 hours NO oxidation.

Publications

J. Gopakumar, P.M. Benum, I.-H. Svenum, B.C. Enger, D. Waller, M. Rønning: X-ray spectroscopy experiments unravel the transformations of ruthenium catalysts during nitric acid production, ERSF News, Spotlight on science, 2024 February 19

J. Gopakumar, P.M. Benum, I.-H. Svenum, B.C. Enger, D. Waller, M. Rønning: Redox transformations of Ru catalyst during NO oxidation at industrial nitric acid production conditions, 2023, J. Chem. Eng. 475, 146406.

iCSI moments 2023

Skiing day in March

Grenoble in July

New PhDs: Wei, Karoline and Monica

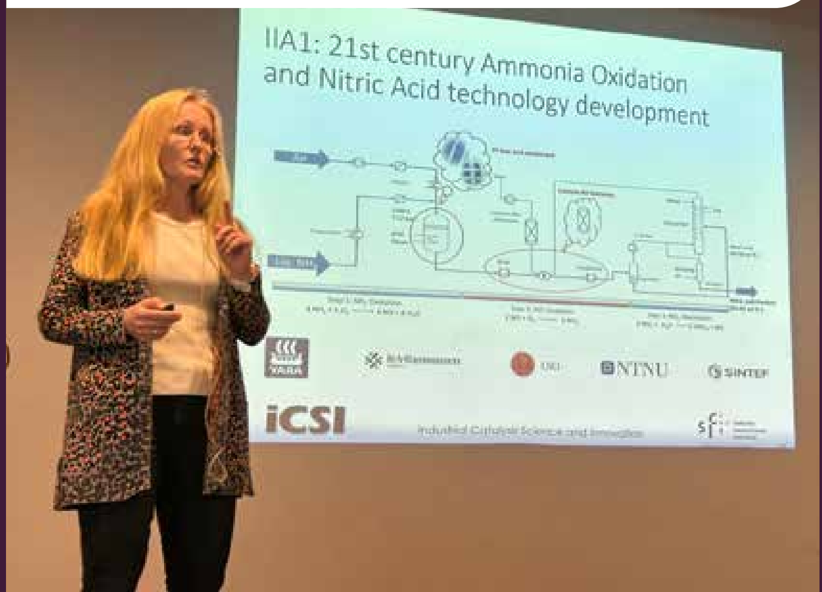
The red sweather team

Engineers have fun

Daily life in Chemistry building 5

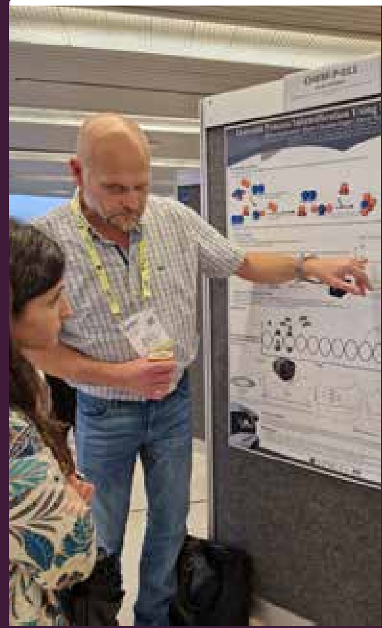
Hilde invited to a sushi dinner during the seminar in June

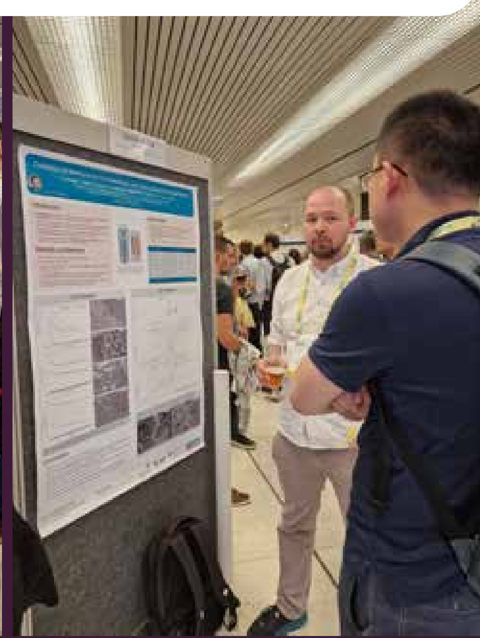
Hyfer seminar in September



Project meetings with Dynea and KAR

Europacat 2023, In Prague in August





iCSI Concluding Seminar

The last annual iCSI seminar was set up to be partly overlapping with a seminar for our international CATHEX partners. As a result, a total of 70 catalysis researchers from three continents could gather to share results and discuss catalytic challenges. It was especially appreciated that the two scientific advisors Enrique Iglesia and Alessandra Beretta had opportunity to join the event. The seminar, summing up eight years of hard work in the SFI, took place in the chemistry buildings at NTNU over the course of four days in June.

The first day was internal for iCSI and was set aside for project managers and industry partners who summarised the main achievements in the six different Industrial Innovation Areas and what the industry has gained from participation in the SFI.

On the following Tuesday, there were scientific presentations by iCSI PhD candidates and members of the scientific advisory committee, as well as nice words from the dean of the Faculty of Natural Sciences and the Research Council of Norway. Centre director Hilde Johnsen Venvik gave an overview of her experiences, while a former iCSI PhD candidate showed us a glimpse of his career after iCSI and his new employer CoorsTek. The day was finalized with a celebration dinner at the NINA restaurant

The event continued on the Wednesday with lectures from the guest CATHEX professors from Madison, Cape Town, Oslo, Shanghai and Toronto, as well as iCSI postdocs. The final day was filled with short lectures from PhD candidates and postdocs from NTNU and Madison, Cape Town and Toronto. Both Tuesday and Wednesday ended with a poster session where the discussions continued.

*From the left: **Top row:** Jasmina Hafizovic Cavka, Manos Mavrikakis, Aase Marie Hundere, Pablo Beato. **Mid row:** Alessandra Beretta, Enrique Inglesia and Jithin Gopakumar, William Broomhead, Jia Yang and De Chen. **Bottom row:** Sushi dinner at Hilde's Garden and CATHEX dinner at Ladekaia. Photos: Anne Hoff*







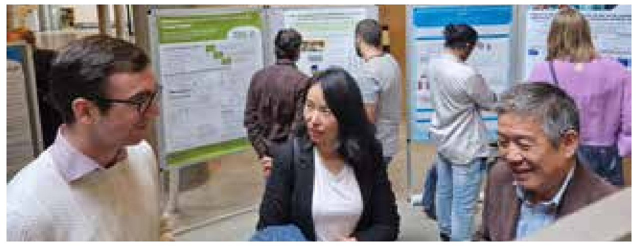


Photo: Per Henning

Program for the iCSI/CATHEX seminar in Trondheim June 5-8 2023.

Day 1	Monday June 5 iCSI seminar, Room R9, NTNU	
Time	**Who**	**Topic**
12:00-13:00	Lunch@Realfagskantina	
13:00-13:15	Pablo Beato, Topsøe, Chair of the iCSI Board	Welcome to seminar
13:15-13:40	IIA1: Anja O. Sjåstad, UiO and David Waller, Yara	Main achievements in research and innovation
13:40-14:00	IIA2: Silje F. Håkonsen, SINTEF and Karl Isak Skau, Yara	
14:00-14:25	IIA3: Jasmina H. Cavka, SINTEF, Ole Bjørkedal Håvik, Dynea and Ann Kristin Lagmannsveen, K. A. Rasmussen	
14:25-14:45	Coffee break	
14:45-15:10	IIA4: De Chen, NTNU	Main achievements in research and innovation
15:10-15:35	IIA5: Stian Svelle, Univ. of Oslo	
15:35-16:00	IIA6: Magnus Rønning, NTNU	
18-22	Casual dining @Hilde's garden in Sleipnes vei 5	

Day 2	Tuesday June 6 iCSI seminar, guest from CATHEX are welcome to join, Room R9, NTNU	
Time	**Who**	**Topic**
09:00-09:10	Edd Blekkan, NTNU	Welcome
09:10-09:30	Jithin Gopakumar, NTNU	Ruthenium catalysts to attain NO-NO_2 equilibria at Industrial nitric acid conditions
09:30-09:50	Wei Zhang, NTNU	Mechanism and Kinetic Studies of Ethylene Oxychlorination to Ethylene Dichloride and Vinyl Chloride
09:50-10:05	Youri van Valen, NTNUw	Effects of Co-feeding reactants in H_2 and CO oxidation over Silver
10:05-10:20		
10:20-10:50	Coffee break	
10:50-11:10	Bjørn Gading Solemsli, Univ. of Oslo	Methylation versus oligomerization of light Alkenes and Benzene through stepwise reaction with Methane in Cu-Exchanged Zeolites.
11:10-11:25	Dimitrios Pappas, CoorsTek	Experiences after iCSI
11:25-11:40	Aase Marie Hundere, RCN	Words from the Research Council of Norway
11:40-11:55	Øyvind Weiby Gregersen, NTNU	Words from Dean of NV faculty
12:00-13:00	Lunch@ Realfagskantina	
13:00-13:30	Hilde j. Venvik, iCSI director	iCSI experiences and achievements
13:30-14:20	Prof. Enrique Iglesia, Univ. of Califor-nia, Berkeley, iCSI scientific advisor	Uncovering active sites and reaction channels in C-H activation reactions on oxide catalysts
14:20-14:40	Coffee break	
14:40-15:30	Prof. Alessandra Beretta, Politecnico di Milano, iCSI scientific advisor	NH_3 catalytic cracking: kinetic investigation over Ru-supported cat-alysts and reactor study with thermally and electrically conductive structured internals
15:30-15:40	Short break	
15:40-15:55	Bjørn Christian Enger, SINTEF	Catalysis needs for the future (Outlook to 2030)
15:55-16:00	Pablo Beato, Topsøe	Concluding remarks
16:00-16:30	Break	
16:30-17:30	All	iCSI & CATHEX Poster session
19-24	Celebration dinner@NINA-kantina	

Day 3	Wednesday June 7 CATHEX/iCSI seminar, Room R9, NTNU	
Time	**Who**	**Topic**
09:00-09:10	Ingeborg-Helene Svenum, NTNU	Welcome
09:10-09:50	Jia Yang, Shanghai Jiao Tong Univ.	Iron based Fischer Tropsch synthesis
09:50-10:30	Manos Mavrikakis, Univ. of Wisconsin-Madison	Challenging well-established assumptions for the active site in heterogeneous catalysis
10:30-11:00	Coffee break	
11:00-11:20	Tina Bergh, iCSI@NTNU	Developing transmission electron microscopy methods for catalyst characterisation at NTNU
11:20-12:00	Cathy Chin, Univ. of Toronto	Catalytic Transformation of Light Alkane and Alkanol Feedstock
12:00-13:00	Lunch@ Realfagskantina	
13:00-13:40	Patricia Kooyman, Univ. of Cape Town	Removal of CO from H_2
13:40-14:20	Anja O. Sjåstad, Univ. of Oslo	On the ammonia oxidation reaction
14:20-14:40	Coffee break	
14:40-15:20	Michael Claeys, Univ. of Cape Town	Direct CO_2 hydrogenation for the production of sustainable fuels and chemicals
15:20-15:40	Huong Lan Huynh, Best Catalysis PhD, Norwegian Chemical Society	CO_2 methanation on Ni-Fe based catalysts: mechanistic and structured reactor study
15:40-16:00	Sebastian Prodinger, iCSI@UiO	Developing Synthesis-Structure-Activity Relationships for the Partial Oxidation of Methane: Achievements and Outlook
16:00-16:30	Break	
16:30-17:30	All	iCSI & CATHEX Poster session

Day 4	Thursday June 8, CATHEX young researchers day, seniors are welcome to join, Room R9	
Time	**Who**	**Topic**
09:00-09:10	Petter Tingelstad, NTNU	Welcome
09:10-09:40	Prof. Magnus Rønning, NTNU	Lessions learned from operando characterisation of catalysts in demanding sample environments
09:40-09:50	Ask lysne, NTNU	Hydrotalcite-Derived Nickel-Cobalt Catalysts for Steam Reforming of Bio-Syngas Hydrocarbon Impurities
09:50-10:00	Oscar Luis Ivanez Encinas, NTNU	Poisoning of cobalt based catalysts in FT
10:00-10:10	Thulani Nyath, Univ. of Cape Town	Manganese-cobalt oxide $[(Mn_xCo_{1-x})_3O_4]$ catalysts studied in situ during the preferential oxidation of carbon monoxide
10:10-10:20	Bjørn Baumgarten, NTNU	Reducing coking by coupling CO_2 Hydrogenation and MTO
10:20-10:40	Coffee break with discusions	
10:40-10:50	Ainara Moral Larrasoana, NTNU	Dechlorination of plastic waste derived pyrolysis oil
10:50-11:10	Guangming Cai, Univ. of Toronto	Consequences of Site Correlations and Structural Dynamics on Metal Oxides for C−O Formation and C−H Scission
11:10-11:30	William Broomhead, Univ. of Toronto	Catalytic Significance of the Oxide-Support Interface in Alkanol Oxidative Dehydrogenation
11:30-11:50	Coffee break with discusions	
11:50-12:00	Felix Herold, NTNU	Controlled Doping of Carbon Catalyst Supports by Atomic Replace-ment via Gasification-Assisted Heteroatom Doping
12:00-12:10	Evangelos Smith, Univ. of Wiscon-sin-Madison	Reactive liquid crystals for the design of chemoresponsive hydro-gen sensors
12:10-12:20	Monica Pazos Urrea, NTNU	Utilizing carbon nanofiber-supported catalysts for hydrogen pro-duction via aqueous phase reforming of ethylene glycol
12:20-12:30	Albert Miro í Rovira, NTNU	Hydrodeoxygenation of bio-oil
12:30-13:30	Lunch	
13:30	Social activities (optional)	

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
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, 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 WP4.4 WP4.5	NTNU, SINTEF, INEOS Inovyn
IIA5	The next step in direct activation of lower alkanes	WP5.1 WP5.2 WP5.3	TOPSOE, SINTEF, UiO University of Oslo
IIA6	Generic projects for additional industrial synergies	WP6.1 WP6.2 WP6.3 WP6.4 WP6.5 WP6.6 WP6.7	NTNU, UiO University of Oslo, dynea, SINTEF, INEOS Inovyn, TOPSOE, YARA

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

The IIA1 team 2023

Anja Olafsen Sjåstad	UiO	IIA leader, PhD supervisor and WP responsible (WP1.1), advisor (WP1.2)
Helmer Fjellvåg	UiO	Advisor (WP1.1-1.2)
Julie Hessevik	UiO	PhD candidate (WP1.1)
Martin Jensen	UiO	Researcher (WP1.1)
Henrik Sønsteby	UiO	Researcher (WP1.1)
Cathinka S. Carlsen	UiO	Master's student (WP1.1)
David Waller	YARA	Industry senior researcher (WP1.1-1.2-1.3), PhD supervisor (WP1.1)
Daniela Farmer	YARA	Industry researcher (WP 1.1)
Oskar Iveland	YARA	Industry researcher (WP 1.1)
Marianne S. Grønvold	YARA	Industry researcher (WP 1.1)
Torgeir Lunde	YARA	Industry senior
Ann Kristin Lagmannsveen	KA Rasmussen	Industry Researcher (WP1.1-1.2)
Federica Mudu	KA Rasmussen	Industry Researcher (WP1.1-1.2)
Silje Fosse Håkonsen	SINTEF	Researcher WP responsible (WP1.2)
Børge Holme	SINTEF	Researcher (WP1.2)
Martin F. Sunding	SINTEF	Researcher (WP1.2)
Kari Anne Andreassen	SINTEF	Senior Engineer (WP1.2)
Joanna Pierchala	SINTEF	Research engineer (WP1.2)
Magnus Rønning	NTNU	PhD supervisor, WP responsible (WP1.3)
Jithin Gopakumar	NTNU	PhD candidate (WP1.3)
Pål Martin Benum	NTNU	Master's student (WP1.3)
Rune Lødeng	SINTEF	PhD supervisor, senior researcher (WP1.3)
Bjørn Christian Enger	SINTEF	Senior researcher (WP1.3)

Experimental investigations of Pt/PtRh volatilisation and catchment

The Ostwald process, where ammonia is oxidised to form nitric oxide, is a key step in producing mineral fertilisers. A net made of PtRh alloy is used to efficiently catalyse the reaction with very high yields of NO. Due to the harsh environment, some of the Pt is lost during the process as $PtO_2(g)$. A PdNi net downstream the catalyst will catch most of the lost Pt. However, during operation, the catchment nets reconstruct and swell, ultimately leading to a high pressure drop over the reactor. In addition, some of the Pd is lost from the catchment nets. Research carried out by UiO and Yara has showed that the catchment net reconstructs regardless of Pt catchment or not. In the work reported below, we wanted to further study which gas phase species are responsible for Pd reconstruction and perhaps also Pd loss.

A set of washed and woven Pd nets was exposed to a gas flow at ambient pressure and 920°C, using different gas phase species and concentrations, and time on stream. The degree of reconstruction of the surface and the cross-sections of the net wires was subsequently analysed by scanning electron microscopy (SEM).

Initial results showed that exposure to NO or NH_3 over 10 days on stream causes heavy reconstruction. Cross-section of wires from selected experiments are shown in Figure 1. The images clearly show that when either NO or NH_3 was present, the original dense Pd wires have

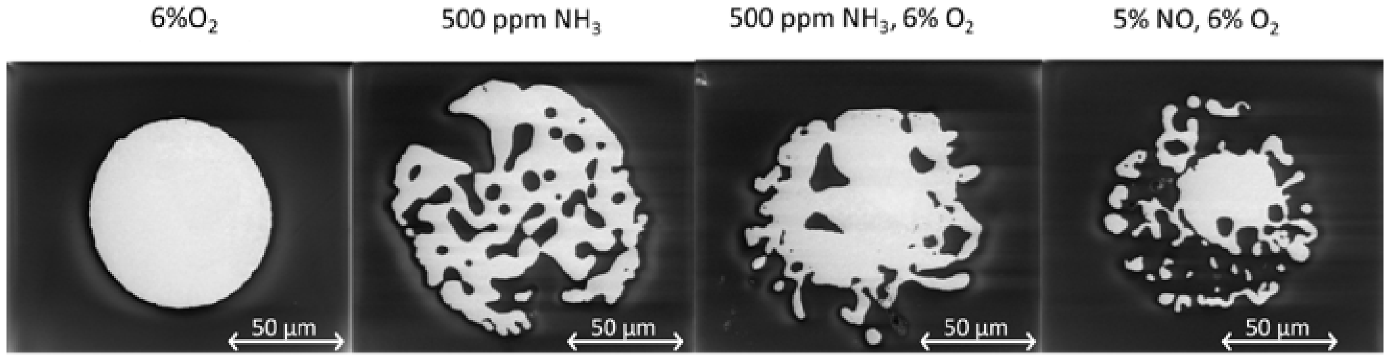


Figure 1 SEM images of Pd wire cross-sections after being exposed to O_2, NH_3, NH_3 + O_2 or NO + O_2 in N_2 for 10 days on stream at 920°C.

swollen. The diameter has increased and there is reconstruction through the entire wire. Where the fresh wire had a smooth surface, the treated wires now have a more sponge-like appearance. The reconstruction in the three experiments have much of the same characteristics and severity.

Figure 2 displays wire cross-sections from experiments conducted using a flow of 5% NO in nitrogen at 920°C for 24 hours with (top) and without (bottom) 6% O_2 added. The results reveal that oxygen has a strong inhibiting effect on the reconstruction of palladium the NO induces. The wires simultaneously exposed to NO and O_2 have developed some fine porosity along the outer surface after 24 hours. In one of the wires investigated (top right), bands of larger pores have also developed deeper into the core, most likely along grain boundaries. The wires exposed to NO without O_2 show more severe reconstruction after 24 hours. The reconstruction is often complete throughout the wires (bottom right), while a small solid core can be observed at other locations (bottom left). As in industrially used Pd(Ni) nets, there is massive swelling. One hypothesis for the reconstruction of Pd due to NO is that NO adsorption on the Pd surface leads to recrystallisation. In the presence of O_2, competitive adsorption thus inhibits the NO adsorption and recrystallisation.

Overall, these results show that the Pd nets reconstruct even after very short times on stream considering the total length of a catchment net campaign. Interestingly, the nets reconstruct in the presence of product gas alone (without Pt catchment) and the surface layer seems to completely re-crystallise, attacking first in the grain boundaries. Crystallites of Pd have been recovered just downstream the Pd net, showing that at least some of the Pd loss observed from the nets in these experiments is due to mechanical loss.

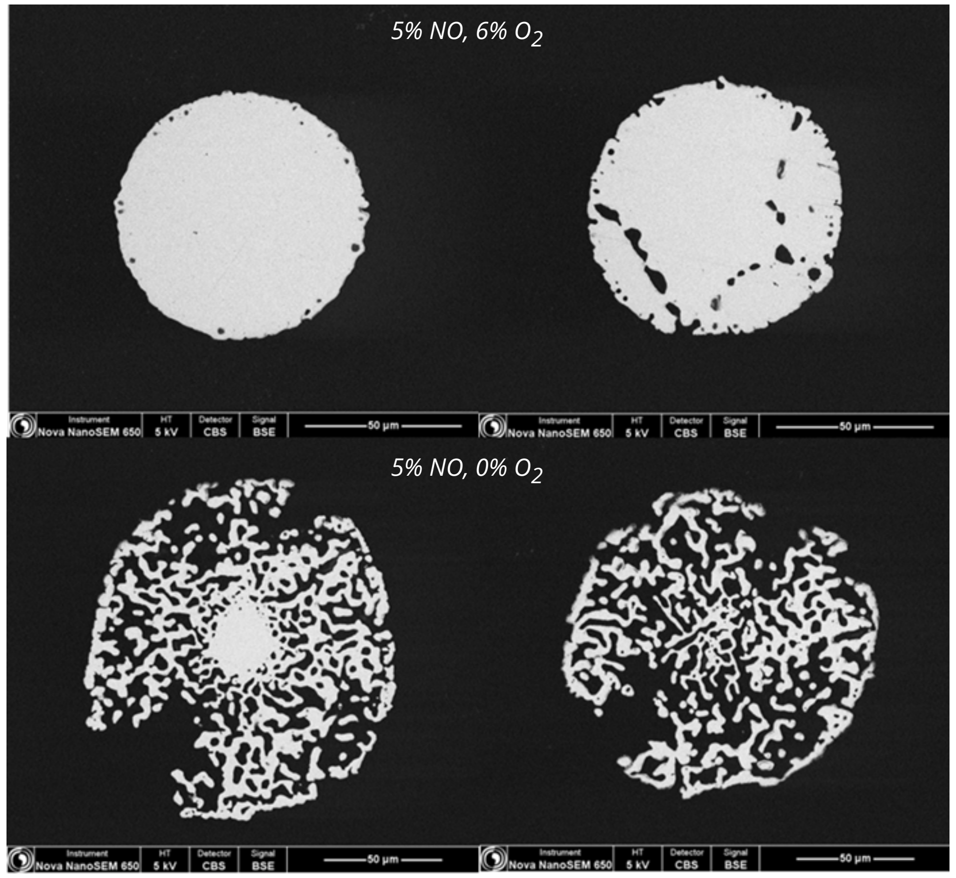
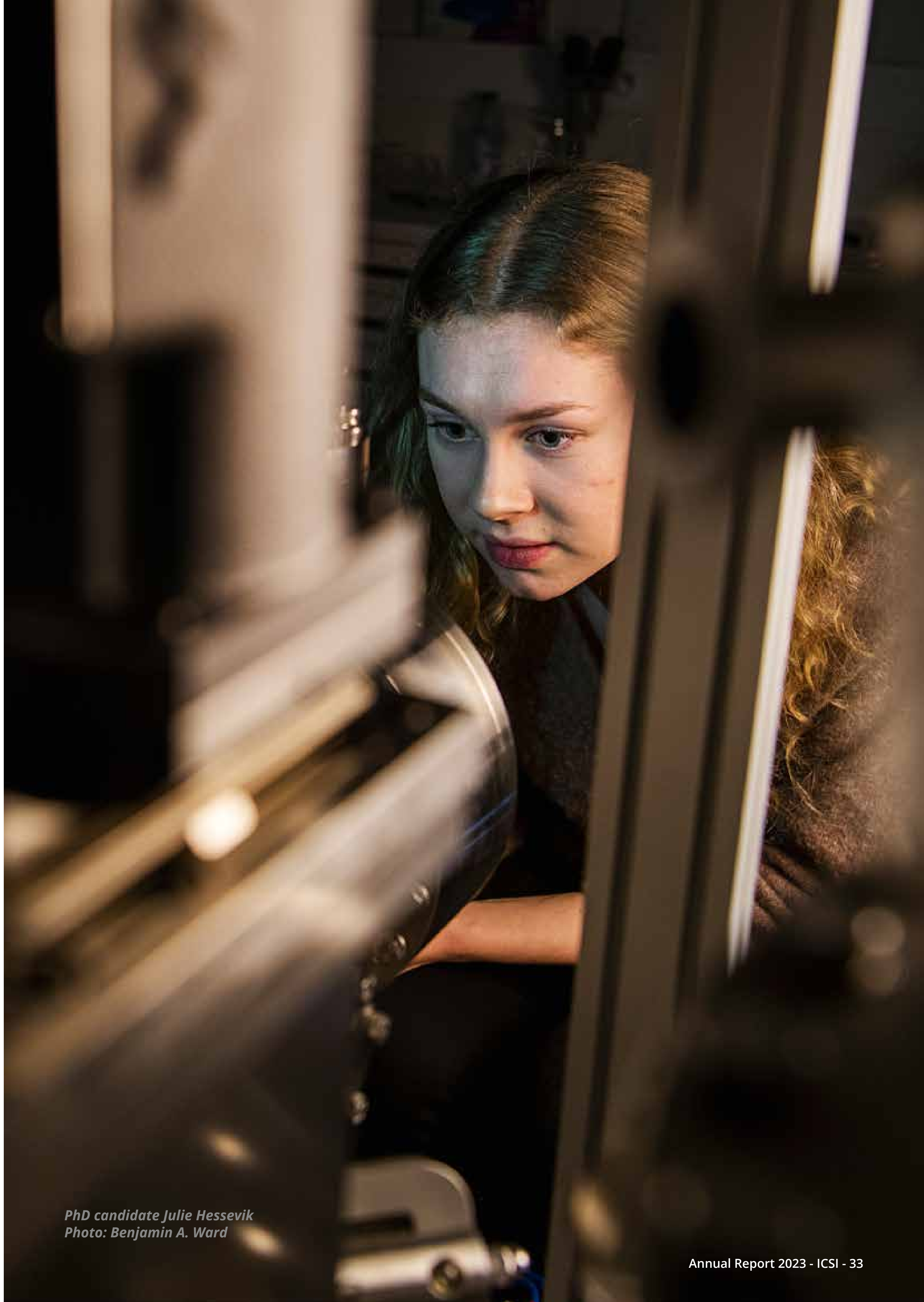


Figure 2 SEM images of cross-sections of Pd wires after being exposed to 5% NO in N_2 for 24 hours at 920°C. In the presence of oxygen (top) and without oxygen (bottom).

Publication

Publications and conference contributions from IIA1 in 2023 are listed on page 58.



PhD candidate Julie Hessevik
Photo: Benjamin A. Ward

IIA2: Abatement of Nitrogen-containing Pollutants – State-of-the-art Catalyst Technology

The IIA2 team 2023

Jasmina Hafizovic Cavka	SINTEF	IIA leader
David Waller	YARA	Industry senior researcher
Karl-Isak Skau	YARA	Industry researcher
Siri-Mette Olsen	YARA	Industry researcher
Silje F. Håkonsen	SINTEF	Researcher and WP responsible
Martin F. Sunding	SINTEF	Researcher
Patricia Almeida Carvalho	SINTEF	Senior researcher
Anna Lind	SINTEF	Researcher

Motivation

When ammonia is combusted in a nitric acid plant in the Oswald process to produce NOx, N_2O is an unwanted bi-product. The levels of N_2O might appear to be low but the high Global Warming Potential (GWP) of N_2O of 298 means that it used to account for 50% of Yara's Greenhouse Gas (GHG) emissions. For this reason, Yara developed an abatement catalyst that is located directly below the platinum-based oxidation catalysts. The catalyst consists of a

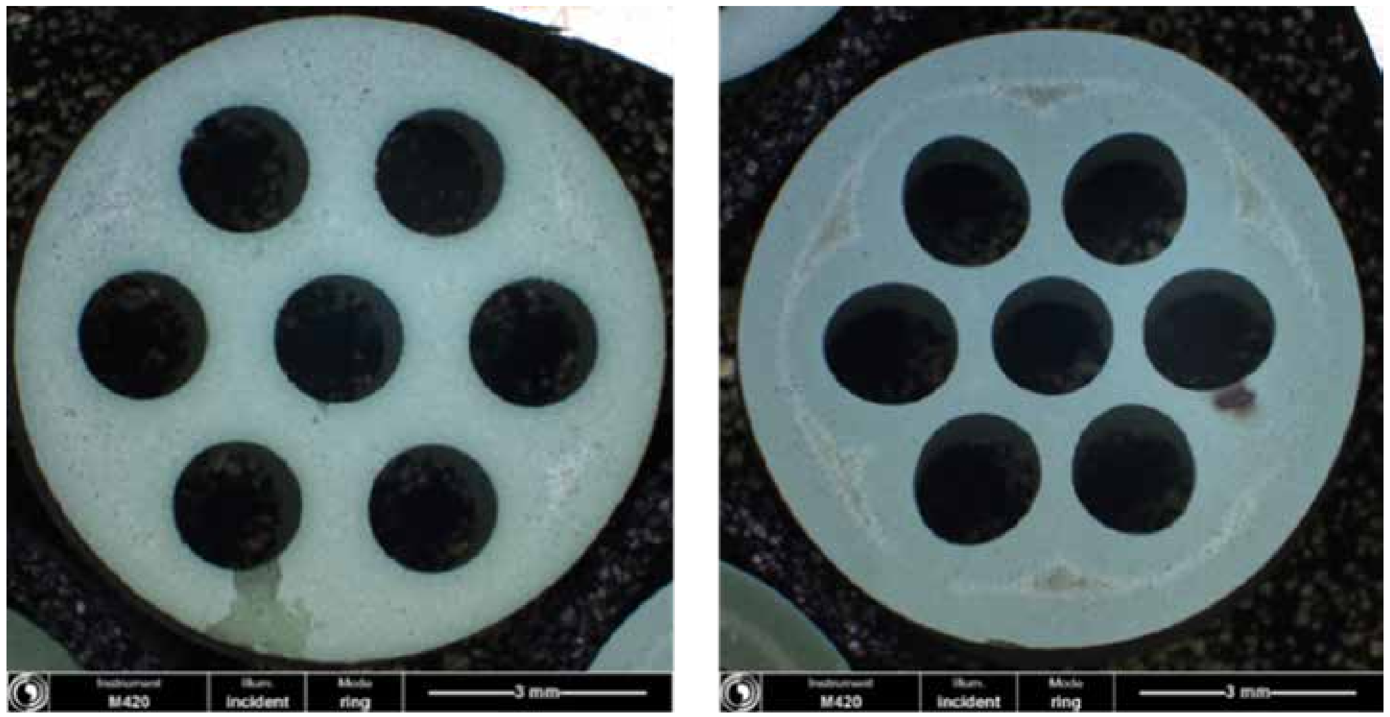


Figure 1 Light microscopy. Used catalyst (left) and used, reformed catalyst (right).

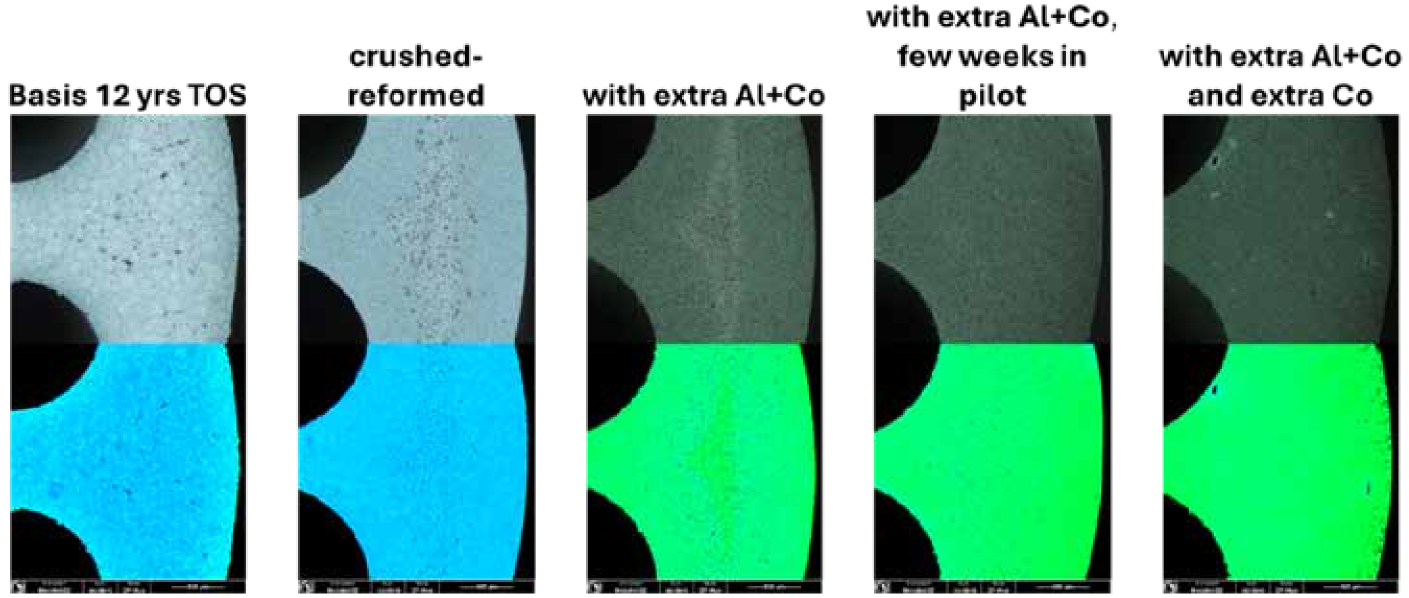


Figure 2 Light microscopy, dark field illumination of polished cross-sections of the used and reformed catalysts. Top row: Standard colours. Bottom row: hue.

Co and Al spinel phase supported on CeO_2. This catalyst can achieve > 95% abatement with no changes to plant operation. The deN_2O catalysts have proven to be able to perform at a high level in the harsh conditions inside an ammonia burner for over a decade. In this project, aged catalyst is studied to better understand the transitions in the catalyst with the aim to formulate an even more active and stable catalyst.

Research project

A deN_2O catalyst that has been in operation in a commercial nitric acid plant for 12 years has been reformed/reshaped by crushing and extrudation, and active materials have been added. These catalysts have been investigated by light microscopy and SEM-EDS.

Polished cross-sections of the samples were investigated using light microscopy, dark field illumination. By emphasising the colour using the hue in HSL (hue-saturation-lightness), it highlights the change in colour in the samples.

Previous iCSI results have proven that a blue colour indicates a catalyst depleted in cobalt, with a spinel phase of $CoAl_2O_4$, while a green colour indicates the spinel phase Co_2AlO_4. Figure 2 shows that the catalyst that has been 12 years on stream has a homogeneous blue colour through the cross-section, while the reformed catalysts, where additional Co and Al have been added, show a green colour, similar to fresh catalyst samples.

SEM images of the original and reformed catalysts (Figure 3) show that the microstructure is highly similar in the two catalysts.

SEM-EDS of the reformed catalysts with Al and Co additions also show highly similar microstructure to the original catalyst. It confirms an increase in Co, but reveals that the addition of Co is not evenly distributed.

Publication

Conference contributions from IIA2 are listed on page 59.

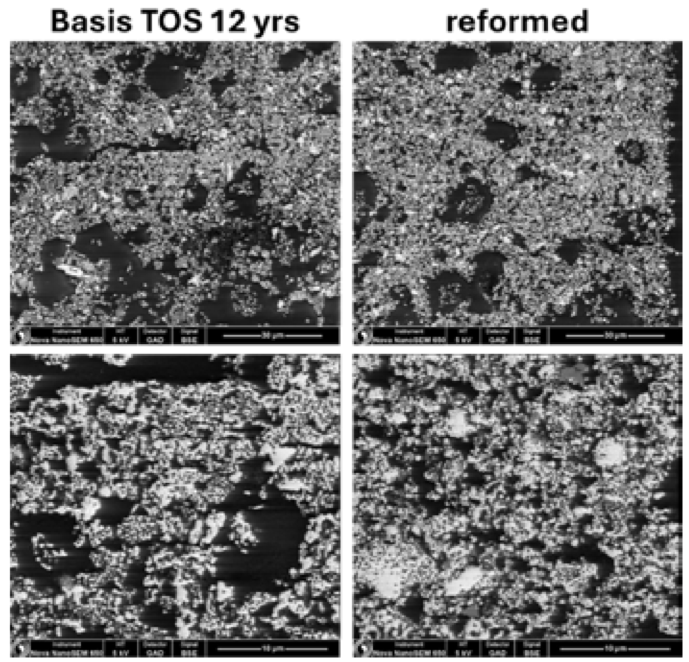


Figure 3 SEM images of a catalyst that has been 12 years on stream (left) and the reformed catalyst (right).

IIA3: Frontier Formalin Technology Development

The IIA3 team 2023

Jasmina Hafizovic Cavka	SINTEF	IIA leader
Hilde Venvik	NTNU	PhD supervisor, WP responsible (WP3.1), advisor (WP3.3)
Jia Yang	NTNU	PhD co-supervisor (WP3.1), advisor (WP3.3)
Youri van Valen	NTNU	PhD candidate (WP3.1)
Matilde Emanuelli	NTNU	Exchange bachelor's student (WP3.1)
Tina Bergh	NTNU	Postdoctoral fellow (WP3.1/WP6.7)
Tomasz Skrzydlo	NTNU	Master's student (WP3.1)
Ann Kristin Lagmannsveen	KA Rasmussen	Industry researcher (WP3.1)
Federica Mudu	KA Rasmussen	Industry researcher (WP3.1)
Ole H. Bjørkedal	DYNEA	Industry researcher (WP3.1-3.2-3.3), WP responsible (WP3.2)
Lars Axelsen	DYNEA	Industry senior (WP3.1-3.2)
Rune Lødeng	SINTEF	PhD co-supervisor (WP3.1), senior researcher (WP3.2-3.3)
Roman Tschentscher	SINTEF	Senior researcher (WP3.2-3.3)
Kari Anne Andreassen	SINTEF	Senior engineer (WP3.3)

Beneath the silver surface – using focused ion beam and electron microscopy to study silver catalysts in 3D.

In IIA3, we study annular and particulate silver catalysts used for the partial oxidation of methanol (CH_3OH) and its relevant sub-reactions, for example oxidation of CO and H_2. The silver surface morphology changes drastically during interactions with oxygen and hydrogen at high temperatures (≳600 °C), which impacts both activity and selectivity. The extent of these microstructural changes into the depth of silver has not yet been well described. We image silver catalysts in 3D after oxidation in various reaction atmospheres, using a destructive tomography method available in the focused ion beam (FIB) – scanning electron microscope (SEM). The method is automated and often called slice-and-view, since the FIB is used to mill away thin slices (here 30-50 nm thick), before the SEM is employed to image the freshly polished surfaces, as shown in Figure 1. Figure 1(a) shows a top-view secondary electron (SE) SEM image of an annular silver catalyst after oxidation of CO and H_2 ("syngas"). Surface faceting and large, well-distributed pinholes are visible. A protection layer (PL) is deposited using the FIB-SEM, as shown in (b), before trenches are milled to expose the silver region beneath the surface, as can be seen in top-view in (c) and side-view in (d). Figures 1(e)-(g) show SE SEM images collected during the subsequent slice-and-view routine. Image processing is done to enhance the pore edges, as exemplified in (h). Finally, we plot the (sub-)surface pores in 3D, as shown in (j). Several large, faceted pores can be seen extending beyond 25 µm into the silver. We believe that this is due to the dissolution of oxygen and hydrogen in the silver crystal lattice and their subsequent recombination, together with a high mobility of silver atoms at high temperature. We also compliment the slice-and-view with electron backscatter diffraction (EBSD) data collected at different stages during the milling, to extract the local crystallographic orientation across the polished surfaces. Furthermore, we use the FIB to prepare cross-sectional lamellae for (scanning) transmission electron microscopy (S)TEM studies. The 4D-STEM method scanning precession electron diffraction (SPED) is employed to map the local crystal orientation, as explained further in the iCSI annual report 2022.

Exchange student in IIA3

During the 2023 autumn semester, WP3.1 had the pleasure of hosting Matilde Emanuelli. Matilde is a bachelor student from Università di Bologna and came to NTNU via the Erasmus exchange programme. During her time here, she investigated the restructuring of annular silver catalysts and compared this to restructuring on industrial granular silver catalysts. Over the course of three months, an experimental campaign was conducted using a variety of atmospheres chosen from sub-reactions of the MTF reaction system. As a result of Matilde's work, we now know that the surface restructuring of our annular catalyst is comparable to that of the catalyst used industrially when they are exposed to the same atmospheres and temperatures. Figure 2 shows the silver surface after hydrogen oxidation on (A) the annular catalyst and (B) the granular catalyst. On both catalysts, we can see the characteristic terraces we have earlier observed after hydrogen oxidation. The resulting pinholes also have similar shapes, in line with previous observations. We would like to thank Matilde for her efforts and wish her the best during the continuations of her studies.

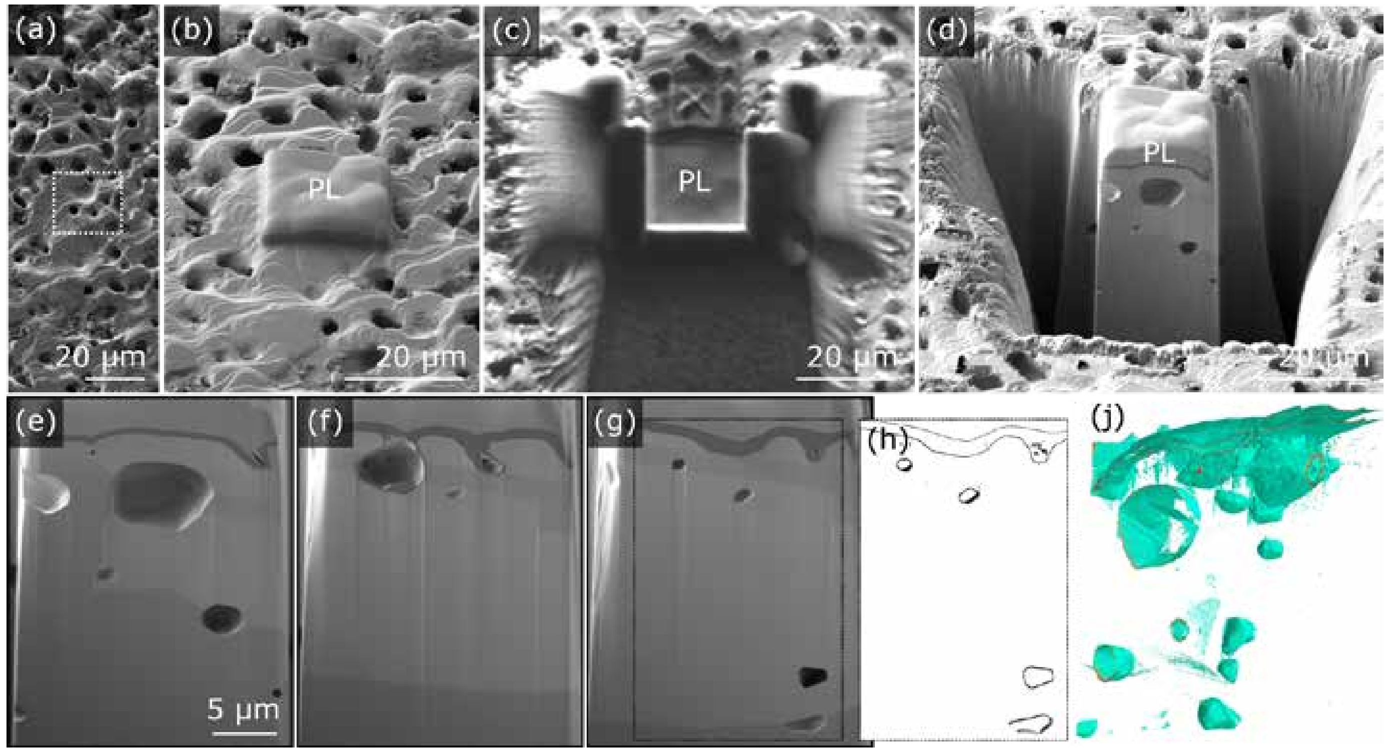


Figure 1 FIB-SEM tomography of an annular silver catalyst after oxidation of syngas. (a) and (b) top-view SE SEM images of the surface before and after deposition of a protection layer (PL). (c) FIB image after milling of trenches. (d) SE SEM side-view image of a milled cross-section. (e)-(g) SE SEM images collected during automated slice-and-view. (h) image processing to enhance the edges in (g). (j) processed slice images plotted in 3D, with the first image shown in (e) pointing to the front left.

Publication

Conference contributions from IIA3 are listed on page 59.

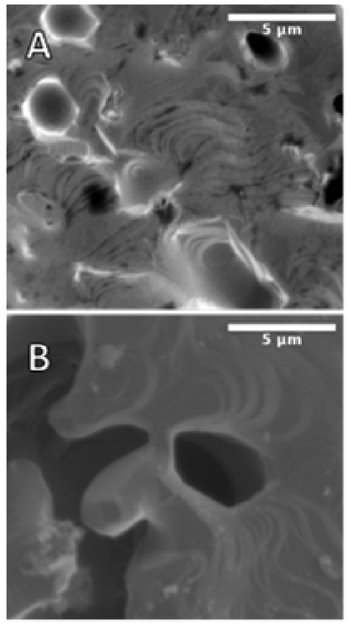


Figure 2 Left: Matilde Emanuelli. Right: SEM images of silver catalysts after hydrogen oxidation; (A) annular catalyst and (B) granular catalyst.

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

The IIA4 team 2023

De Chen	NTNU	IIA leader, PhD supervisor, WP responsible (WP4.2-4.5)
Wei Zhang	NTNU	PhD candidate (WP4.2-4.5)
Lola Irene Stokstad	INEOS Inovyn	Industry researcher (WP4.2-4.5)
Tigran Margossian	INEOS Inovyn	Industry researcher (WP4.2-4.5)
Arne G. Grønvold	INEOS Inovyn	Industry researcher (WP4.2-4.5)
Andrea Marsella	INEOS Inovyn	Industry researcher (WP4.2-4.5)
Vidotto, Sandro	INEOS Inovyn	Industry researcher (WP4.2-4.5)
Macino, Margherita	INEOS Inovyn	Industry researcher (WP4.2-4.5)
Dennis Neu	SINTEF	Researcher (WP4.2, WP4.4)
Torbjørn Gjervan	SINTEF	Researcher (WP4.2)

Kinetic studies on mono-promoter-doped $CuCl_2$/Al_2O_3 catalyst

This study investigates the promoter effects of 14 metal chlorides (NaCl, KCl, RbCl, CsCl, $MgCl_2$, $CaCl_2$, $SrCl_2$, $CeCl_3$, $PrCl_3$, $NdCl_3$, $ErCl_3$, $FeCl_3$, YCl_3, and $SnCl_3$) on the $CuCl_2$/γ-Al_2O_3-based catalysts used for ethylene oxychlorination. It combines transient experiments of the two half-reactions in the redox cycle to understand the effects of different promoters on the reduction and oxidation rates of the catalysts. The results show that promoter doping can tune the redox behaviour of the $CuCl_2$/γ-Al_2O_3-based catalysts and change the rate-determining step (RDS) between reduction and oxidation. All the promoters have a positive effect on the reaction rate at steady-state, but the impact of promoter identity on steady-state $CuCl_2$ concentration varies in accordance with the electronegativity of the promoter metal. This work, summarised in Figure 1, provides a better understanding of the reaction process and mechanism, and highlights the potential of promoter doping for improving the efficiency and stability of $CuCl_2$/γ-Al_2O_3-based catalysts in ethylene oxychlorination. The approach of both transient and steady-state kinetic modelling and simulation is a reliable and efficient method to study promoter effects on reduction-oxidation reactions.

Engineering the Cu oxidation state spatial profile

The understanding of selectivity in heterogeneous catalysis is of paramount importance to society today. Ethylene oxychlorination is a well-developed industrial process, but the selectivity at high conversion needs to be further improved. In this work, we demonstrate the different behaviour of $CuCl_2$/Al_2O_3-based catalysts at a wide conversion range and reveal the importance of spatially distributed $CuCl_2$ concentration for the catalytic performance through the spatial-time resolved UV–vis-NIR approach. A high $CuCl_2$ concentration leads to higher activity, EDC selectivity, and stability. By adjusting the reduction and oxidation potentials within the redox cycle, a spatially distributed high-level oxidation state of Cu was precisely controlled by synergistically coupling $CuCl_2$ with specific promoters. Our engineered, tri-promoter doped KMgLa-$CuCl_2$/γ-Al_2O_3 catalyst exhibits outstanding performance, achieving full conversion with nearly 100% selectivity towards EDC. This study connects catalytic performance to dynamic copper active sites on a spatial scale in real reactions. Understanding this dynamic nature offers fundamental and practical insights, enabling the potential for achieving maximum catalytic performance. See Figure 2 for illustration of mechanism.

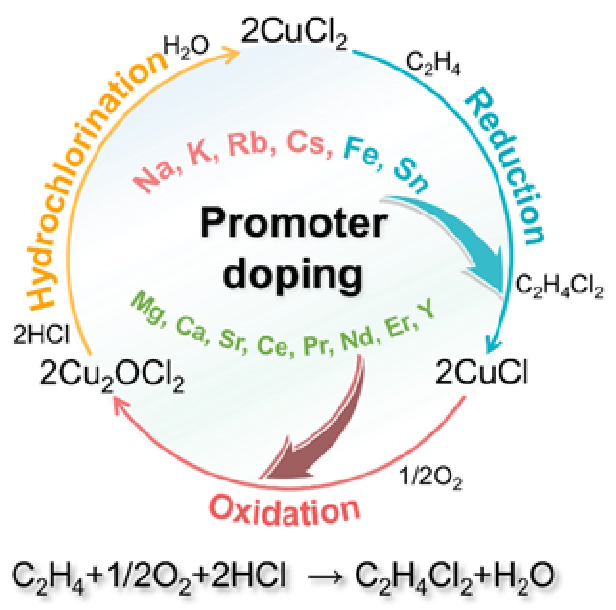


Figure 1 The effects of 14 different metal chloride promoters on the reduction and oxidation steps.

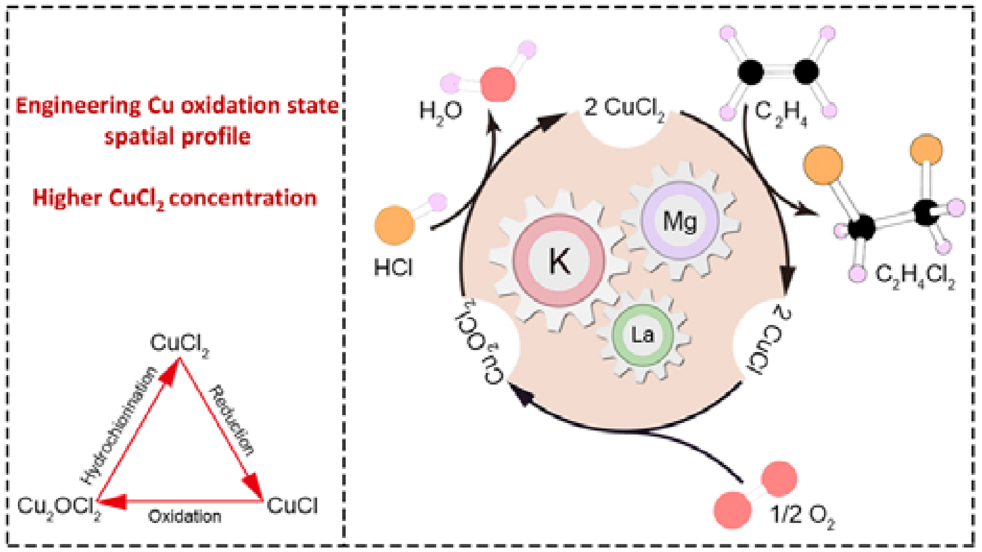


Figure 2 Toward fully selective ethylene oxychlorination through engineering the Cu oxidation state spatial profile.

Multifunctional Pd/N-doped carbon for one-step VCM production

The "seesaw" phenomenon in ethylene oxychlorination and dehydrogenation EDC makes it challenging to maintain high activity simultaneously for the two reactions in one-step VCM production. Conventionally, EDC production proceeds to high yields (90-97%) over $CuCl_2$/γ-Al_2O_3-based catalysts at 220−260°C and low pressure (1−5 bar), characteristic of a highly exothermic reaction. This EDC is subsequently cracked to VCM, endothermically at 500−550 °C and higher pressure (15−20 bar). The VCM selectivity exceeds 90%, but the conversion remains at around 50%. This is an energy-intensive process.

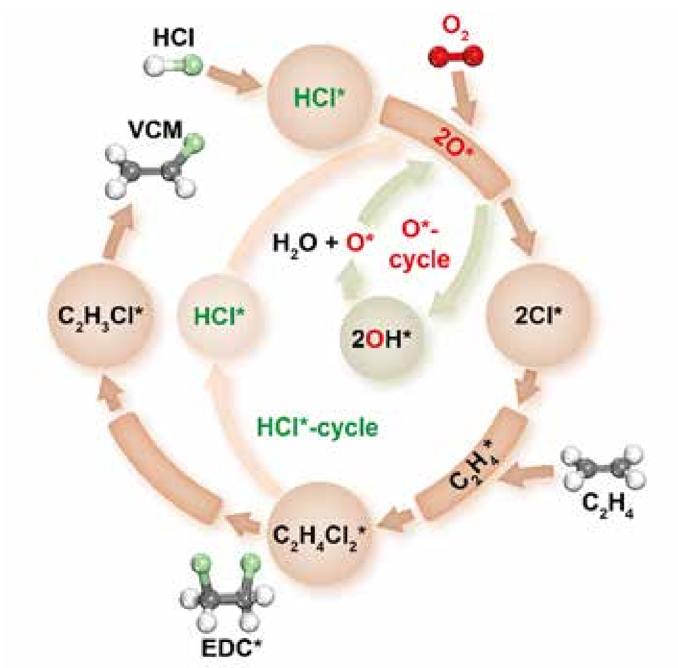


Figure 3 Illustration of the reaction pathway for VCM production via tandem oxychlorination-dehydrochlorination reaction in Pd/NC catalyst.

We recently demonstrated an integrated process in which a nitrogen-doped carbon-supported Pd catalyst (Pd/NC) directly produces vinyl chloride monomer (VCM) from a tandem oxychlorination-dehydrochlorination reaction (Figure 3). Pd/NC led to a VCM yield of above ~50% in a single pass at mild conditions of 250 °C and 1 bar, outperforming the best-reported single process systems and comparable to the industrial two-step method. Pd and NC cooperate to enhance the activity of ethylene oxychlorination and dehydrochlorination to VCM, with multiple reactions involved in a complex reaction network over the catalyst. A new reaction mechanism is proposed that involves recycle of O* and Cl* on the surface. HCl is dissociated with O* and the formed Cl* can directly react with C_2H_4* forming C_2H_4Cl* (EDC*). The adsorbed EDC* prefers to undergo the dehydrochlorination reaction to VCM* and HCl*, which can continue to react in the next cycle with O*. This work highlights how rational design of a multifunctional N-doped carbon-supported Pd catalyst, based on deep understanding of complex reaction mechanisms, leads to unprecedented performance in one-step VCM production.

Publication

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

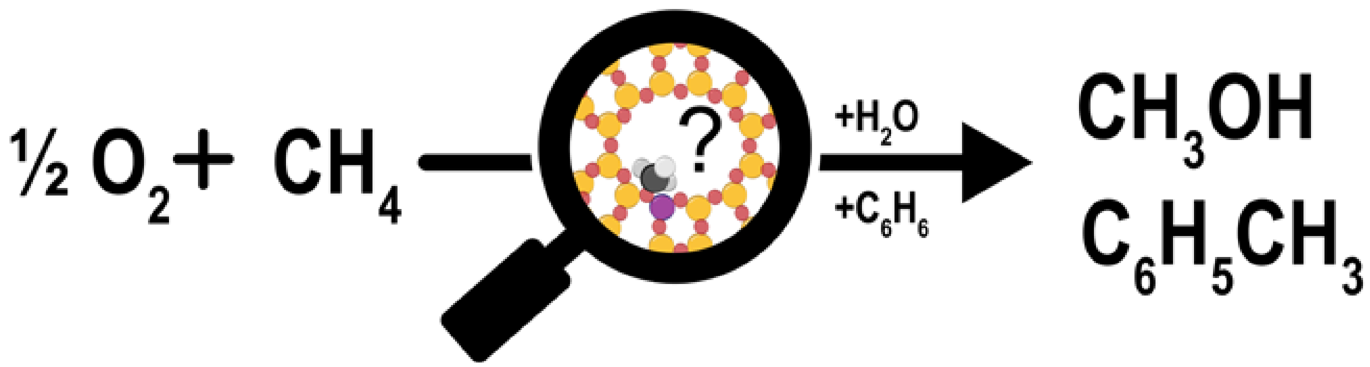
IIA5: The Next Step in Direct Activation of Lower Alkanes

The IIA5 team 2023

Stian Svelle	UiO	IIA Leader, PhD supervisor, WP responsible (WP5.1-5.2-5.3)
Unni Olsbye	UiO	PhD supervisor (WP5.1-5.2)
Karoline Kvande	UiO	PhD candidate (WP5.1-5.2)
Sebastian Prodinger	UiO	Postdoctoral fellow (WP5.1-5.2-5.3)
Bjørn Gading Solemsli	UiO	PhD candidate (WP5.1-5.2)
Izar Capel Berdiell	UiO	Researcher (WP5.1-5.2)
Torstein Fjermestad	UiO	Postdoctoral fellow (WP5.1-5.2)
Pablo Beato	Haldor Topsøe A/S	Industry senior and researcher (WP5.1-5.2-5.3)
Lars Fahl Lundegaard	Haldor Topsøe A/S	Industry researcher (WP5.1-5.2-5.3)
Søren Birk Rasmussen	Haldor Topsøe A/S	Industry senior researcher (WP5.1-5.2-5.3)
Aino Nielsen	Haldor Topsøe A/S	Industry researcher (WP5.1-5.2-5.3)
Mette Christensen Nielsen	Haldor Topsøe A/S	Industry researcher (WP5.1-5.2-5.3)
Hanne Zingler Stummann	Haldor Topsøe A/S	Industry researcher (WP5.1-5.2-5.3)
Bjørnar Arstad	SINTEF	Senior researcher (WP5.3)

2023 marks the last year of full scientific activities in IIA5. Even so, we have still made significant scientific discoveries through the work of PhD candidate Bjørn Gading Solemsli, who will defend his thesis in the first half of 2024.

A major challenge in the stepwise conversion of methane to methanol over Cu loaded zeolites – the main scientific topic of IIA5 – has been to identify the key surface bound methoxy intermediate. Extensive attempts have been made using FT-IR, but to no avail. NMR spectroscopy has provided some insights (Michael Dyballa et al. Zeolite surface methoxy groups as key intermediates in the stepwise conversion of methane to methanol, , ChemCatlChem, (2019), 11, 5022-5026.), but these experiments are always carried out under conditions far from those applied in the actual reaction.



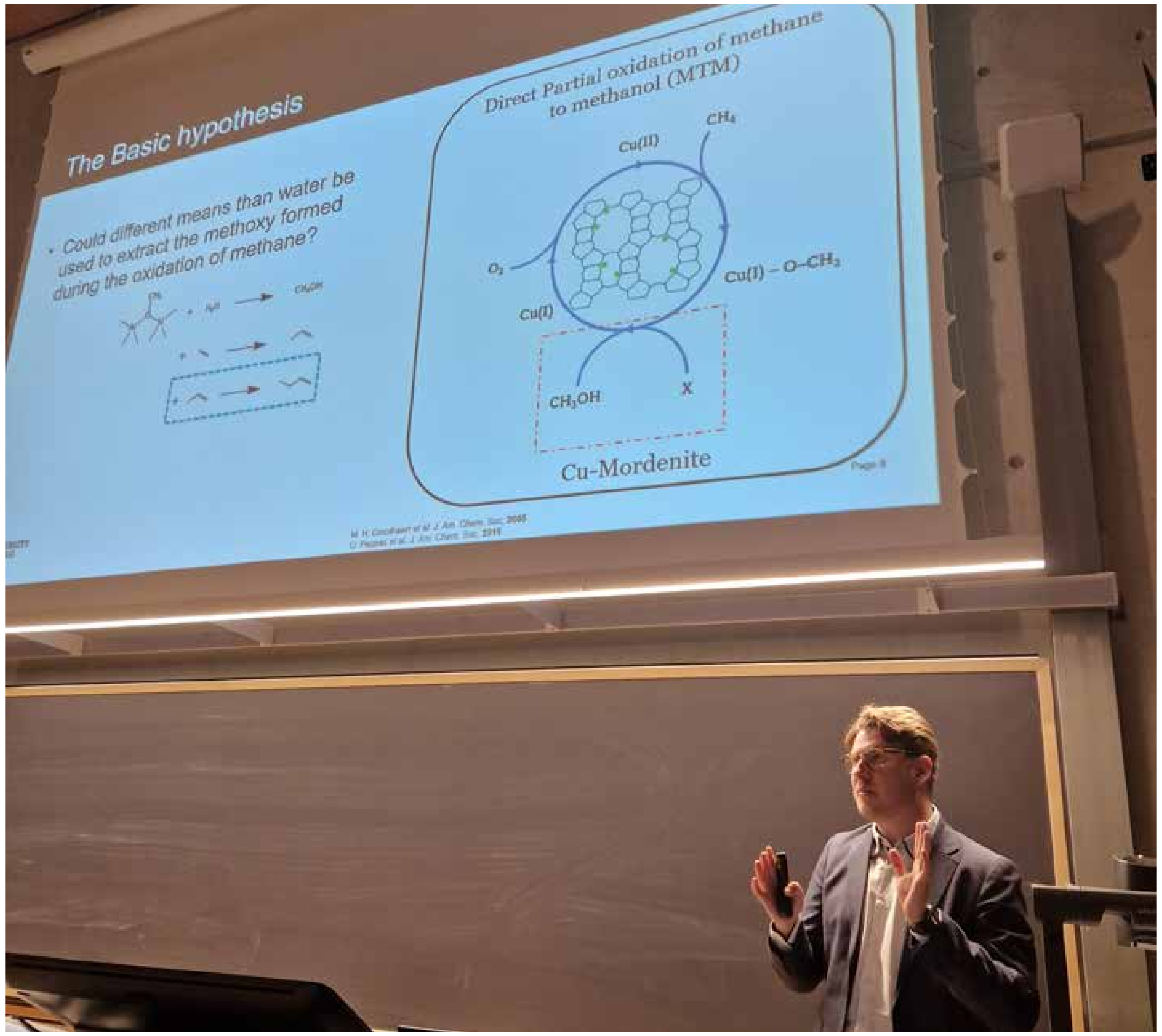
Now you see me, now you don't! By using benzene rather than steam/H_2O, it was possible to detect and quantify the key surface bound methoxy group intermediate in the stepwise conversion of methane to methanol over copper loaded zeolites.

This year, we have employed a novel approach to indirectly observe and quantify the key intermediate under realistic reaction conditions (Bjørn Gading Solemsli et al. Reactivity of Methoxy species towards Methylation and Oligomerization in Cu-Zeolite systems, Catalysis Today (2024) submitted). We have elucidated the reactivity of the methoxy species formed upon C-H activation of methane over copper(II)-oxo species, with various hydrocarbons. Through meticulous experimentation and analysis, we investigated the behaviour of ethylene, propylene, and benzene as reactants for extracting methoxy intermediate species. Results show that benzene undergoes successful methylation, yielding toluene as the sole product, whereas ethylene and propylene reactions are dominated by the oligomerization-cracking pathway. The benzene experiment thus constitutes a direct link to the elusive surface bound methoxy species.

Furthermore, reactions with benzene reveal that only a fraction of the methoxy species are available to react with benzene, and that Brønsted acid sites are needed to facilitate the methylation reaction. By comparing the yield of toluene upon extraction with benzene to the yield of methanol after extraction with steam, we propose a [Methylated Product] : [Methoxy] Ratio (MPMR) as a valuable indicator of the accessibility of methoxy species, but also as an indicator of the nature of the methoxy species. In this study, we have shown the presence of more than one type of methoxy species, being distinguished by either type or accessibility.

Publications

Publications and conference contributions from IIA5 are listed on page 59.



PhD candidate Bjørn Gading Solemsli presenting his results at the iCSI/CATHEX seminar in June 2023.

IIA 6: Generic Projects for Additional Industrial Synergies

The IIA6 team 2023

Magnus Rønning	NTNU	IIA leader, PhD supervisor and WP responsible (WP6.1)
Hilde Johnsen Venvik	NTNU	PhD co-supervisor (WP6.1) and postdoc supervisor (WP6.7)
Samuel K. Regli	NTNU	PhD candidate (WP6.1)
Anja Olafsen Sjåstad	UiO	WP responsible (WP6.2)
Martin Jensen	UiO	PhD candidate, associated (WP6.2)
Mathilde Ingeborg N. Verne	UiO	Master's student (WP6.2)
Evgeniy Redekop	UiO	Researcher (WP6.2)
David Waller	YARA	Industry senior researcher (WP6.2)
Bjørn Christian Enger	SINTEF	WP responsible and senior researcher (WP6.4)
Ingeborg-Helene Svenum	SINTEF	Researcher (WP6.4)
Edd A. Blekkan	NTNU	WP responsible (WP6.5) and PhD supervisor (WP6.5) and co-supervidsor (WP6.6)
Jia Yang	NTNU	WP responsible (WP6.6) and PhD supervisor (WP6.6) and co-supervisor (WP6.5)
De Chen	NTNU	PhD co-supervisor (WP6.5 and 6.6)
Moses Mawanga	NTNU	PhD candidate (WP6.5)
Björn Frederik Baumgarten	NTNU	PhD candidate (WP6.6)
Ingrid Johanne Paulsen	NTNU	Master's student (WP6.6)
Kristin Haukaas Hagen	NTNU	Master's student (WP6.6)
Rune Lødeng	SINTEF	Senior researcher (WP6.6)
Tina Bergh	NTNU	Postdoctoral fellow (WP6.7)

Mapping of stable element distribution in Pt-Rh nanoparticles - In-situ TEM at variable temperature and nanoparticle size

Supported bimetallic Pt-Rh nanoparticles are utilised as catalysts for several important chemical abatement reactions as the ammonia (NH_3) oxidation for NH_3-slip in the maritime sector (diesel engines and the upcoming NH_3 engines). In the development of stable catalytic bimetallic Pt-Rh nanoparticles, full control of the Pt-Rh alloying and know-how about how process temperature, gas atmosphere and nanoparticle size dictate the Pt-Rh element distribution are prerequisites. With this motivation, we mapped the element distribution in Pt-Rh nanoparticles with a 50-50 at.% Pt-Rh versus temperature and nanoparticle size using in-situ TEM (HAADF-STEM) at vacuum conditions.

The in-situ TEM experiments were carried out between room temperature and 650 °C to elucidate the tendency of elemental mixing/segregation with respect to nanoparticle size and temperature for particles ≤ 24 nm. The study fully relies on well-defined 50-50 at. % Pt-Rh solid solution and Rh(core)-Pt(shell) nanoparticles synthesised by means of colloidal routes in our own laboratory (Jensen, M., et al. Innovative approach to controlled Pt–Rh bimetallic nanoparticle ynthesis. RSC Advances, 2022, 12(31), 19717-19725 and Bundli, S., et al., Controlled alloying of Pt-Rh nanoparticles by the polyol approach. Journal of Alloys and Compounds, 2019, 779, 879-885.).

A key finding from the study is that Pt-Rh nanoparticles ≳ 13 nm are stable in a solid solution configuration at high temperatures and in a segregated situation at room temperature. In contrast, Pt-Rh nanoparticles < 13 nm are stable in a solid solution configuration over the entire studied temperature range. This implies there is a nanoparticle size dependent crossover in stable element distribution configuration around 13 nm in the Pt-Rh system at nanoscale. This is a new discovery for the Pt-Rh system, but similar behaviour is observed for some very few other bimetallic systems. The finding is of high value when designing thermodynamic stable nanostructures, and it also demonstrate the need of studying the nanoparticles in-situ rather than using the classic "at birth/post mortem" approach. For more details, see our most recent publication (Jensen, M.,et al., Variable temperature in situ TEM mapping of the thermodynamically stable element distribution in bimetallic Pt–Rh nanoparticles. Nanoscale Advances, 2023, 5(19), 5286-5294).

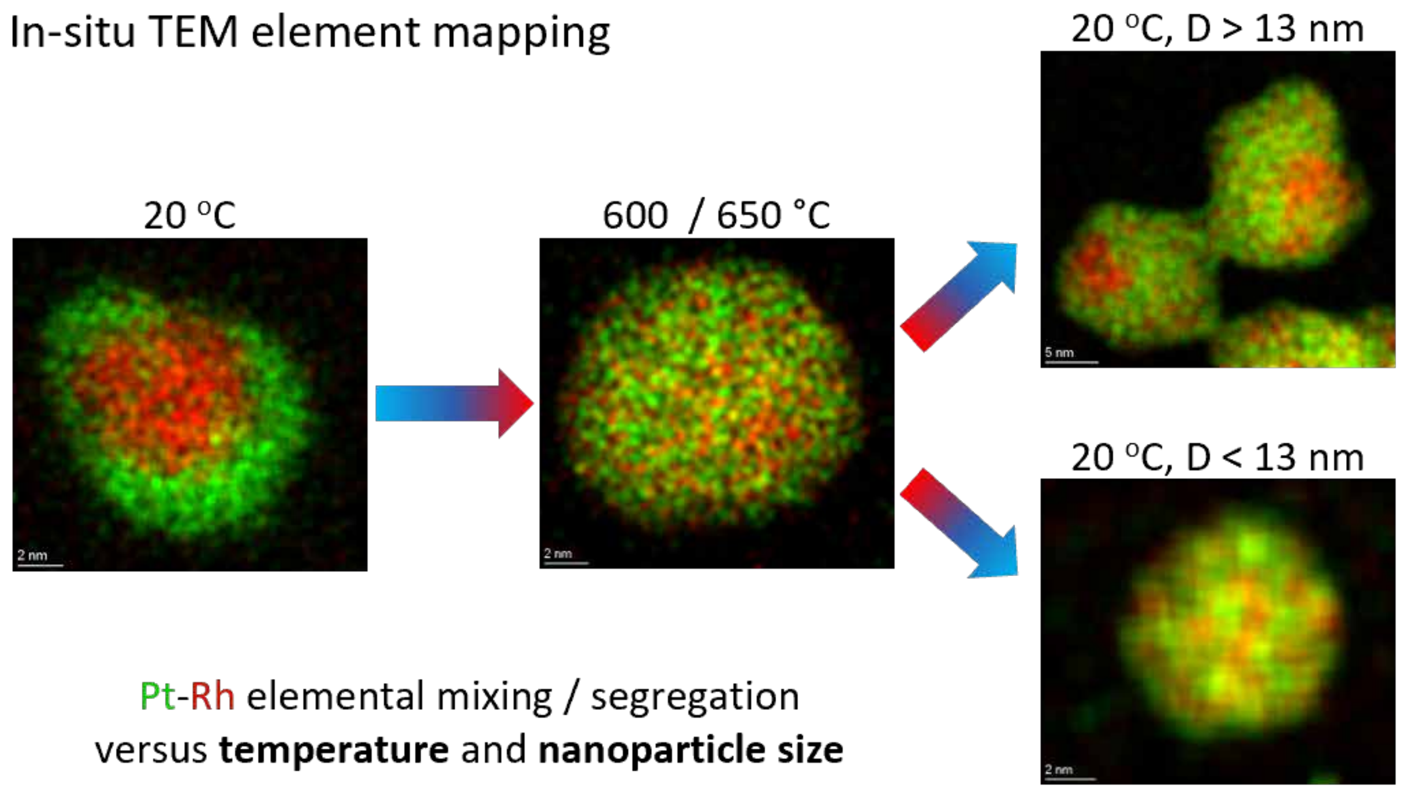


Figure 1 Changes in elemental mixing/segregation when heating and cooling catalysts. Reproduced from M. Jensen, W. Kierulf-Vieira, P. J. Kooyman and A. O. Sjåstad, Nanoscale Adv., 2023, 5, 5286 with permission from the Royal Society of Chemistry.

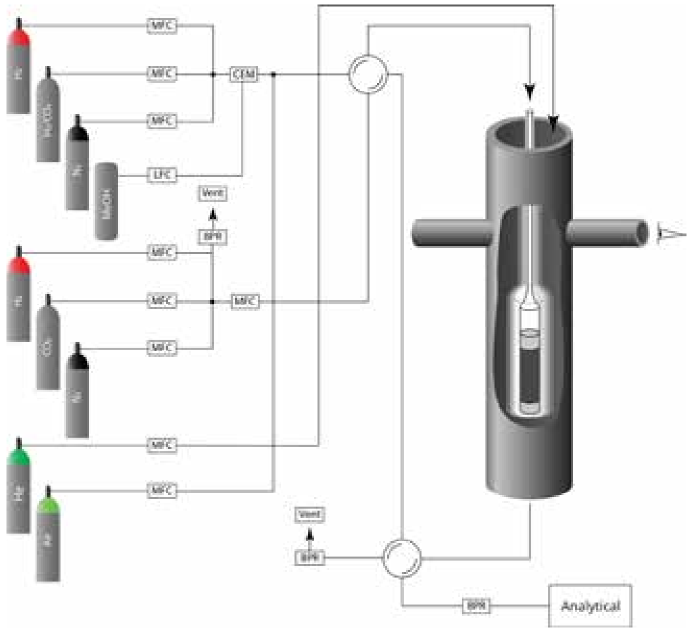


Figure 1 Simplified flowsheet of the ISMA

In-situ analysis of industrial catalytic reactions using a novel ISMA

With the now operational ISMA, weight changes of a catalyst can be measured in operando. This can be caused by coke formation, but also by other deposition or sorption processes. Simultaneously, the product gas composition can be measured using a GC and an MS.

The first reaction examined is the methanol-to-olefins (MTO) reaction using SAPO-34. The MTO reaction is (re-) gaining attention given it can be used to turn green Methanol into more useful olefins, which are the building blocks for many chemical products.

For measurements, the catalyst is placed inside an oscillating quartz element. The element itself is inside an external housing, enabling use at elevated pressures up to 25 bar (Figure 1). Reaction gas can be fed from two independent gas feeding sections, each using up to 3 gases. One of the sections include an evaporator for liquid feed, while the other includes a solution to feed very low flow rates for GHSVs between 500 and 5000 ml/gcatmin.

With changing mass, the frequency changes, and using the formula

$\Delta m = K_o\ [1/f_1^2 - 1/f_0^2]$

the mass of the catalyst can be calculated. Thus, a direct measurement of the mass of the catalyst is possible, without the need to rely on conventional gravimetric microbalances.

In Figure 2, the first results of a MTO reaction are presented. The change of product distribution can be directly related to the amount of coke present on the catalyst.

Additional possible experiments are for example the reduction of catalysts, and the carburization of Fe-catalysts during Fischer-Tropsch experiments.

The ISMA was developed by SINTEF. It is an improved version of the earlier TEOM (Tapered Element Oscillating Mass balance). This project is pioneering and the first to demonstrate the instrument's capabilities under relevant conditions.

Publications

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

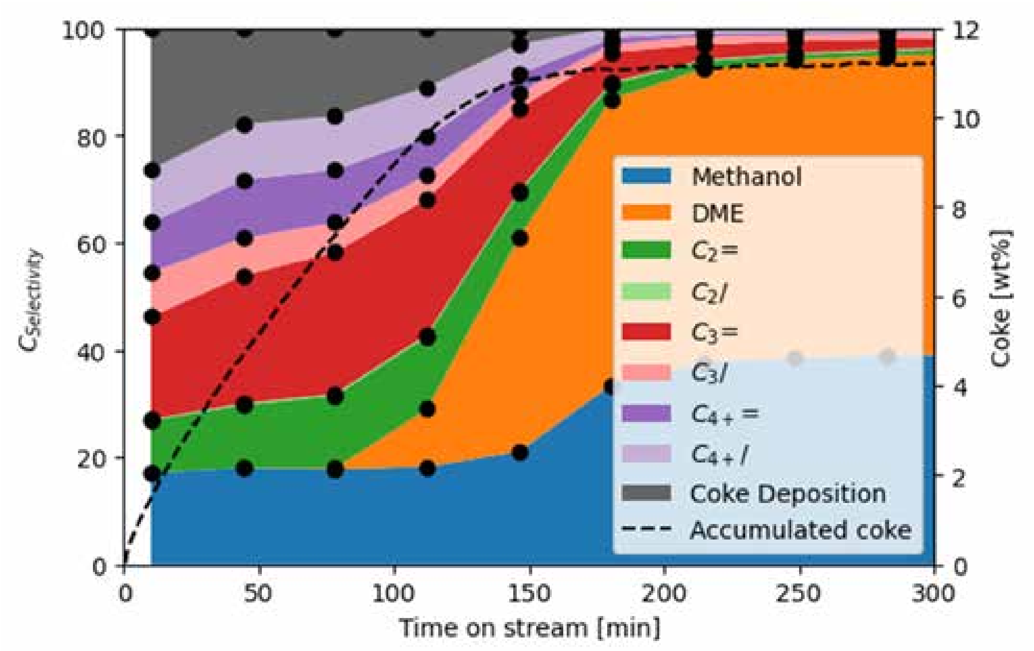
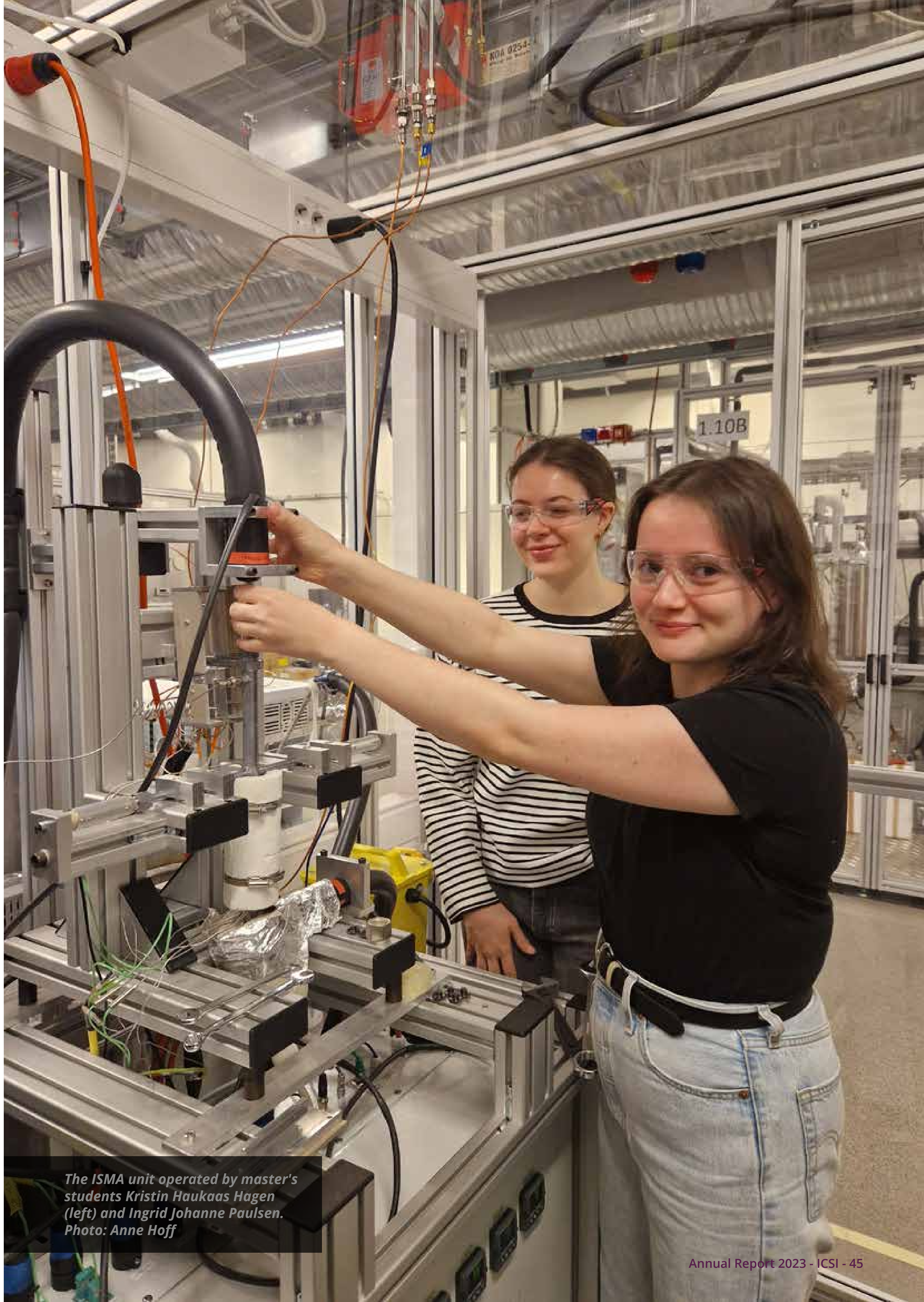


Figure 2: Example Results from an MTO reaction



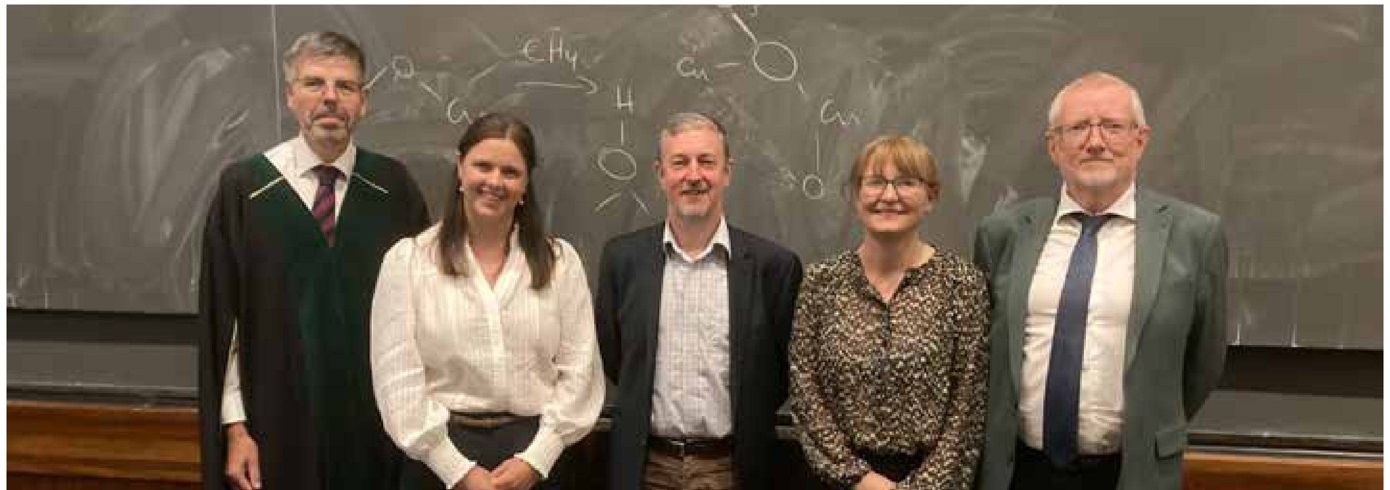
The ISMA unit operated by master's students Kristin Haukaas Hagen (left) and Ingrid Johanne Paulsen. Photo: Anne Hoff

Two New PhDs in 2023

Candidate:	**Karoline Kvande**
Date of defence:	11 August, 2023
Title of thesis:	Compositional and Mechanistic Studies of Cu-zeolites for the Direct Activation of Lower Alkanes
Public trial lecture:	Photocatalysis of methane using non-noble metal oxides
The Committee:	
First opponent:	Professor Andrew Beale Department of Chemistry, University College London, United Kingdom
Second opponent:	Associate Professor Susanne Mossin Department of Chemistry, Technical University of Denmark
Administrator:	Professor Truls Norby Department of Chemistry, University of Oslo, Norway
Supervisor:	Professor Stian Svelle, UiO
Co-supervisors:	Professor Unni Olsbye, UiO, Senior Research Scientist Pablo Beato, Topsoe A/S and Ass. Professor Elisa Borfecchia University of Turin, Italy
iCSI project:	The next step in direct activation of lower alkanes
Industry partner:	Topsoe A/S
Current Position:	Postdoc in Prof. Enrique Iglesia's group University of California, Berkeley, USA

Short summary of thesis

Natural gas and biogas mainly contain small and stable hydrocarbons (light alkanes) and could be a more sustainable resource in the nearest future for the chemical industry, compared to coal and oil. However, due to the stability of alkanes, it is notoriously difficult to make specific products, because, in a reaction, the products are usually more reactive, and unwanted by-products are formed. With the help of activity testing and multiple characterisation techniques, we have obtained insight into a direct, but stepwise pathway to convert alkanes to functionalised products for the industry that is potentially less energy-demanding than the existing ones. The stepwise pathway proceeds over oxidised Cu ions anchored to porous materials (zeolites) that hinder the reactants and products from interacting. With this approach, there is almost no over-oxidation, although the product yield per time from this reaction is low. Accordingly, our focus has been on exploring different parts of the reaction to understand the individual steps and how they can be improved. We have obtained more insight into the Cu speciation and found important activity relationships with both zeolite structure and Cu ion reducibility.



From the left: Prof. Einar Uggerud, PhD Karoline Kvande, Prof. Andrew Beale, Associate Prof. Susanne Mossin and Prof. Truls Norby.

Candidate:	**Wei Zhang**
Date of defence:	17 November, 2023
Title of thesis:	Catalyst Development of Ethylene Oxychlorination to Ethylene Dichloride and Vinyl Chloride
Public trial lecture:	Production of Green Ammonia under Mild Conditions
The Committee:	
First opponent:	Professor Enrico Tronconi, Politecnico di Milano, Italy
Second opponent:	Professor Cathy Chin, University of Toronto, Canada
Administrator:	Dr. He Li, Department of Chemical Engineering, NTNU
Supervisor:	Professor De Chen
Co-supervisors:	Dr. Kumar Ranjan Rout
iCSI project:	PVC Value Chain: World class energy and raw material efficiency for the production of Chlorine and Vinyl Chloride Monomer
Industry partner:	INEOS Inovyn
Current Position:	Temporary researcher position in Catalysis group at Department of Chemical Engineering, NTNU

From the left: Dr He Li, PhD Wei Zhang, Prof. Cathy Chin and Prof. De Chen. Above on the screen: Prof. Enrico Tronconi

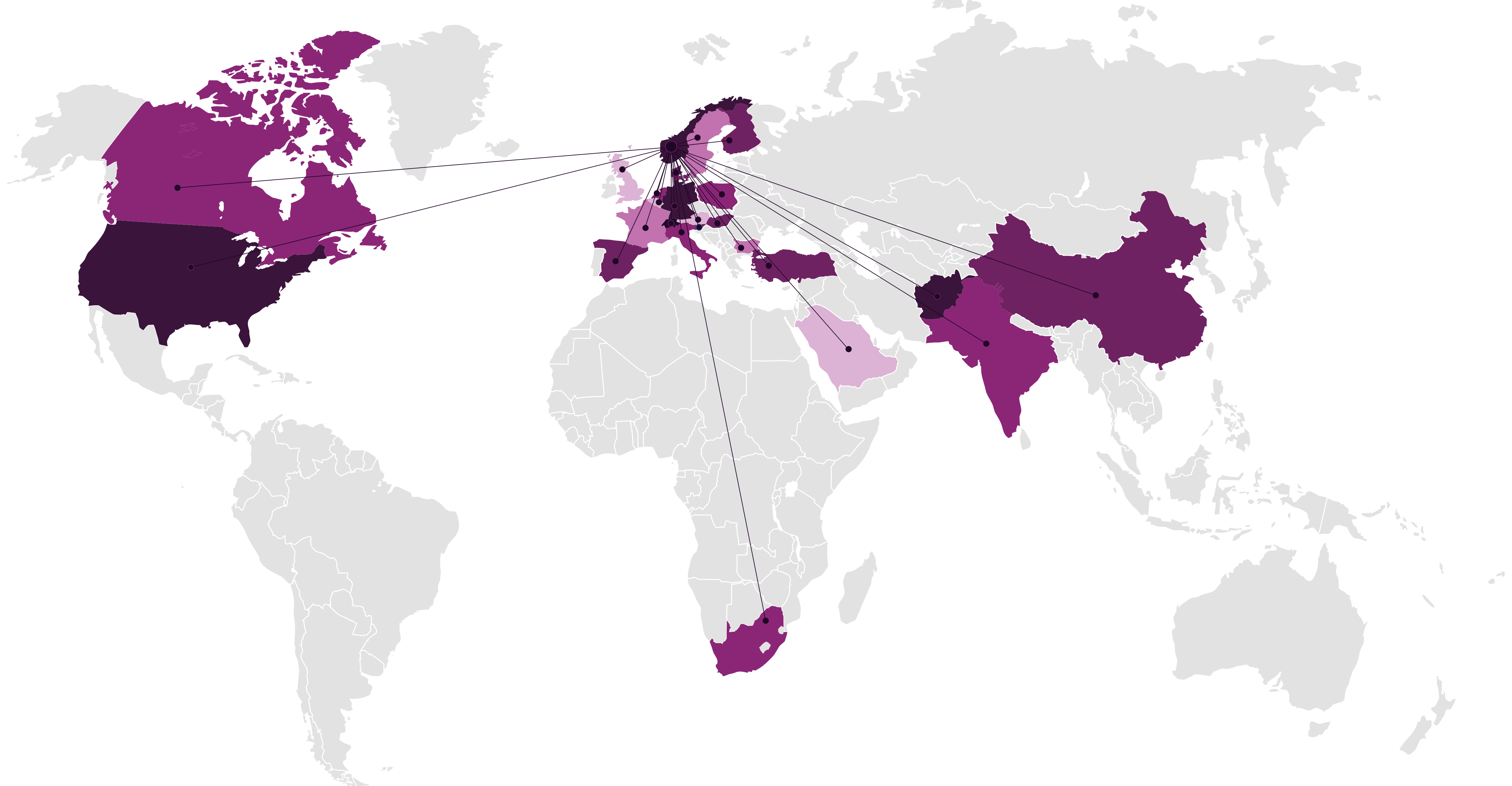
Short summary of thesis

Vinyl chloride monomer (VCM) is a critical component in the production of polyvinyl chloride (PVC), one of the most extensively used plastic polymers, through the polymerisation process. In addition to being an intensive energy consuming process, there are many undesirable products from EDC cracking that can foul the reactor and reduce the product quality. In addition, coke formation at the high-temperature cracker tubes is another main challenge. Efforts to address these challenges using more efficient and sustainable materials and a new route for simplifying the complex process to produce VCM are highly demanded.

The scope of this PhD thesis was to study and gain a better understanding of fundamental reaction mechanisms and the dynamic behaviour of active sites in real reaction conditions by using advanced characterisation technologies and kinetic studies, highlighting the rational catalyst design and new chemistry on the ethylene oxychlorination process and further VCM production.

In this work, the study of ethylene oxychlorination encompasses both fundamental aspects and the exploration of novel chemistry. We strive to enhance the efficiency and sustainability of VCM manufacturing processes, contributing to a more environmentally friendly chemistry.

Internationalization



Hosting a centre like iCSI makes the catalysis community at NTNU and the affiliated research institutions attractive for international students and researchers. However, the number of foreign master's students in the catalysis group at NTNU fell dramatically in the autumn of 2023. The most likely reason for this is the new rules on tuition fees for students coming from outside the EU/EEA. But the catalysis group is still characterised by a very international composition, and the majority of PhD candidates and postdocs are from abroad. The 69 master's students, PhD candidates, postdocs and guest researchers within or affiliated with iCSI represent 17 countries. Non-Norwegians make up 52% of this group of employees and students, which is a decrease from 61% in 2022.

Four exchange PhD candidates visited iCSI in 2023 with stays lasting from 2 weeks up to 6 months. Three master's/bachelor's exchange students were guests of the catalysis group at NTNU. What we have seen is that several of the guest master's students and exchange PhD candidates return as PhD candidates and postdocs, which illustrates the attractiveness of the group. Half of the scientific publications from 2023 were published in collaboration with colleagues at international universities and industry.

The CATHEX project is a network project running from 2020 to 2025. It links iCSI with four world-leading catalysis environments: the University of Cape Town, East China University of Science and Technology (ECUST), University of Toronto and University of Wisconsin-Madison. Both professors and PhD candidates from all the CATHEX partners, excluding ECUST, were present at the combined iCSI/CATHEX seminar in June, contributing with lectures and posters. One professor, one postdoc and one PhD candidate from NTNU/UiO were supported by CATHEX for stays abroad in 2023, while one professor, one PhD candidate and one researcher from the partners were supported for stays in Norway.

Since 2019, iCSI Director Hilde Venvik has been representing Norway in EFCATS (European Federation of Catalysis Societies) as part of the Officers of the Council – and as the Vice President in 2023.

In early 2023, the EFCATS council announced that NTNU in collabaration with all the Nordic catalysis groups will be the host and organisers of EuropaCat 2025. This is the most important meeting place for European catalysis researchers, and as many as 1000 – 1500 participants are expected to visit Trondheim in September 2025.

In 2023, Hilde Venvik finalised the three-year period as Lise Meitner-professor at the Department of Chemical Engineering at Lund University.

Overview of international collaborations:

Universities and Institutes

- *Aalto University, Finland*
- *AGH University of Science and Technology, Poland*
- *Anna University, India*
- *Bulgarian academy of Science, Bulgaria*
- *Cardiff University, United Kingdom*
- *Chalmers University of Technology, Sweden*
- *China University of Petroleum (Huaton), China*
- *CNR, Italy*
- *CSIC, Spain*
- *Centre National de la Recherche Scientifique (CNRS), France*
- *Delft University of Technology, Netherlands*
- *East China University of Science and Technology, China*
- *École Polytechnique Fédérale de Lausanne, Switzerland*
- *ETH Zürich, Switzerland*
- *Ghent University, Belgium*
- *Institut de Recherches sur la Catalyse et l'Environnement de Lyon, CNRS, France*
- *Instituto Nacional del Carbón, INCAR-CSIC, Spain*
- *Karlsruhe Institute of Technology – KIT, Germany*
- *KAUST, Saudi Arabia*
- *Kemijski Institut– NIC, Slovenia*
- *Luleå University of Technology, Sweden*
- *Lund University, Sweden*
- *Manchester Metropolitan University, United Kingdom*
- *MAX-IV Laboratory, Lund, Sweden*
- *Max Planck Institute for Energy Conversion, Germany*
- *Norner Research AS (SCG Chemicals), Norway*
- *Paul Sherrer Institut, Schweiz*
- *Polytechnic University of Catalonia, Spain*
- *Politecnico di Milano, Italy*
- *Research Institutes of Sweden (RISE), Sweden*
- *School of Chemistry and Chemical Engineering, Shanghai Jiao Tong University, China*
- *Shanxi Institute of Coal Chemistry, Chinese Academy of Sciences, (ICC), China*
- *SLAC National Accelerator Laboratory, USA*
- *Sorbonne University, France*
- *Stanford University, California, USA*
- *Swiss-Norwegian Beamlines at ESRF, France*
- *Technical University of Denmark, Denmark*
- *Universidad Del Pais Vasco/ Euskal Herriko Unibertsitatea UPV/EHU, Spain*
- *University of Bologna, Italy*
- *University College London, United Kingdom*
- *University of California, Berkeley, USA*
- *University of Cape Town, South Africa*
- *University of Eastern Finland, Finland*
- *University of Sheffield, United Kingdom*
- *University of Toronto, Canada*
- *University of Turin, Italy*
- *University of Wisconsin-Madison, USA*
- *Utrecht University, Netherlands*

Companies

- *Albemarle, Netherlands*
- *Arkema France SA; France*
- *B.T.G. BV, Netherlands*
- *Borealis Polyolefine, Austria*
- *BTG-BTL, Belgium*
- *C2P2, Lyon (CNRS), France*
- *Elkem Silicon Materials, Norway/France*
- *Equinor, Norway (med?)*
- *Firmenich, Switzerland*
- *ICI Caldaie, Italy*
- *ILS, Integrated Lab Solutions, Germany*
- *Johnson Matthey, United Kingdom*
- *Linde, Germany*
- *Neste, Finland*
- *NextChem SPA, Italy*
- *OMV, Austria*
- *Process design center B.V. (PDC), Netherland*
- *Ranido, Czeck Republic*
- *Repsol SA, Spain*
- *Siemens Energy, Sweden*
- *Steeper, Denmark*
- *Tata Steel UK Limited, UK*
- *Topsoe AS, Denmark*
- *TotalEnergies, France*
- *Turkiye Petrol Rafinerileri Anonim Sirketi (Tüpras),Turkey*
- *UOP LLC, USA*
- *VTT, Finland*

European research - Horizon 2020 and Horizon Europe project

BIKE – BImetallic Catalysts Knowledge-based development for Energy applications. H2020-MSCA-ITN: iCSI-partner involved: NTNU. Duration: 2019-2023.

C123 - Methane oxidative conversion and hydroformylation to propylene. H2020-CE-NMBP-24-2018. iCSI-partner involved: SINTEF(coordinator). Duration: 2019-2023.

COZMOS - CO_2 hydrogenation to light hydrocarbons. H2020-LC-SC3-RIA & H2020-LC-SC3-2018- NZE-CC. iCSI-partners involved: UiO (coordinator), SINTEF, Topsøe. Duration: 2019-2023.

CUBE - Unravelling the secrets of Cu-based catalysts for C-H activation, H2020 ERC-Syg-2019. iCSI-partners involved: UiO (coordinator), duration: 2019-2023

MesoSi-CO_2 – Design of low-cost and carbon-resistant Ni-based mesoporous silicas for chemical CO_2 utilization through tri-reforming of methane. H2020-MSCA-IF: iCSI-partner involved: NTNU. Duration: 2020-2024

EBIO - Turning low value crude bio liquids into sustainable road transport fuels. H2020-EU.3.3.2., iCSI-partner involved: SINTEF (coordinator). Duration: 2020-2024

EHLCATHOL - Chemical transformation of enzymatic hydrolysis lignin (EHL) with catalytic solvolysis to fuel commodities under mild conditions. H2020-LC-SC3-RES-1-2019. iCSI-partner involved: NTNU. Duration: 2020-2024

Unravelling the secrets of Cu-based catalysts for C-H activation. ERC-SYNERGY. iCSI-partner involved: UiO. Other Norwegian partners: NMBU, International partners: Max-Planck, University of Turin. Duration: 2020-2026

PyroCO_2 - Demonstrating sustainable value creation from industrial CO_2 by its thermophilic microbial conversion into acetone. LC-GD-3-1-2020. iCSI-partner involved: SINTEF. Duration: 2021-2026.

OPTIMAL - Smart and CO_2 neutral Olefin Production by arTificial Intelligence and MAchine Learning. H2020-MSCA-RISE-2020. iCSI-partners involved: NTNU, SINTEF. Duration: 2022-2024

ēQATOR - Electrically heated catalytic reforming reactors. HORIZON-CL4-2021-RESILIANCE-01-14, iCSI partner involved: SINTEF, Duration: 2022 – 2025

TUNEMOF - Metallolinker-Functionalized MOF Catalysts for CO_2 Hydrogenation , HORIZON-MSCA-2021-PF-01 , iCSI-partners involved: UiO, Topsøe, Duration: 2022-2025

H4C Europe - Building a European Community of Practice of Hubs for Circularity. HORIZON-CL4-2021-TWIN-TRANSITION-01-1, iCSI-partners involved: SINTEF, Duration: 2022-2026

REFOLUTION - Refinery integration, scale-up and certification for aviation and marine biofuels production, HORIZON-CL5-2022-D3-01-01, iCSI-partners involved: SINTEF (coordinator), Duration: 2022-2026

HYPER - An electrochemically produced oxidiser for modular, onsite generation of HYdrogen PERoxide, HORIZON-CL4-2022-TWIN-TRANSITION-01-, iCSI-partners involved: SINTEF (coordinator), Duration: 2022-2026

DEMO - Discovery of efficient Enzyme-like Metal Organic frameworks to activate biomethane at low temperature, HORIZON MSCA Joint doctoral network, iCSI-partners involved: UiO, Duration: 2023-2027

CompSci - Training in Computational Sciences, HORIZON 2020 MSCA COFUND. iCSI-partners involved: UiO (coordinator), duration: 2021-2026work, iCSI-partners involved: UiO, Duration: 2023-2027

International collaborations supported by RCN and sources other than EU

Bio4Fuels - Norwegian Centre for Sustainable Bio-based Fuels and Energy. Centre for Environment-friendly Energy Research (FME, 257622), iCSI-partners involved: SINTEF, NTNU. International partners: Haldor Topsøe, Johnson Matthey, Duration: 2016 – 2024

TESFun- Theoretical and Experimental Study and Research on Functional Materials (DIKU)., iCSI-partner involved: UiO. International partner: University of Anna, India, Duration 2017-2023.

CO_2LO - Conversion of CO_2 to light olefins by cascade reactions over bifunctional nanocatalysts. iCSI-partner involved: UiO. International partners: University of Torino, The laboratory of Chemistry, Catalysis, Polymers and Process (C2P2). Funding source: NFR, Nano 2021. Duration 2019-2023

CCU-Net - Material technologies for post-combustion CO_2 capture and utilization network. Call for proposals involving Nordic or Nordic-Baltic PhD and researcher mobility. iCSI-partner involved: UiO. International partners: DTU, Luleå University of Technology, University of Eastern Finland. Duration: 2020-2024

TOMOCAT - Tracking the deactivation of shaped zeolite catalysts in time and space using X-ray diffraction tomography. iCSI-partner involved: UiO. International partners: Topsøe, University of Torino. Funding source: NFR, Forskerprosjekt (FRIPRO) Nano 2021. Duration 2020-2024.

CATHEX - Advances in heterogeneous catalysis through integrated theoretical and experimental efforts. RCN – INTPART iCSI-partners involved: NTNU, UiO. International partners: University of Cape Town, University of Toronto, University of Wisconsin-Madison, East China University of Sci. & Techn., Duration: 2020-2025

PhotoRed – Photoelectrochemical carbon dioxide reduction. EØS-Poland. iCSI-partner involved: SINTEF Industry. Other Norwegian partners: SINTEF Ocean, University of South Eastern Norway. International partners: West Pomeranian University of Technology. Duration: 2021-2023

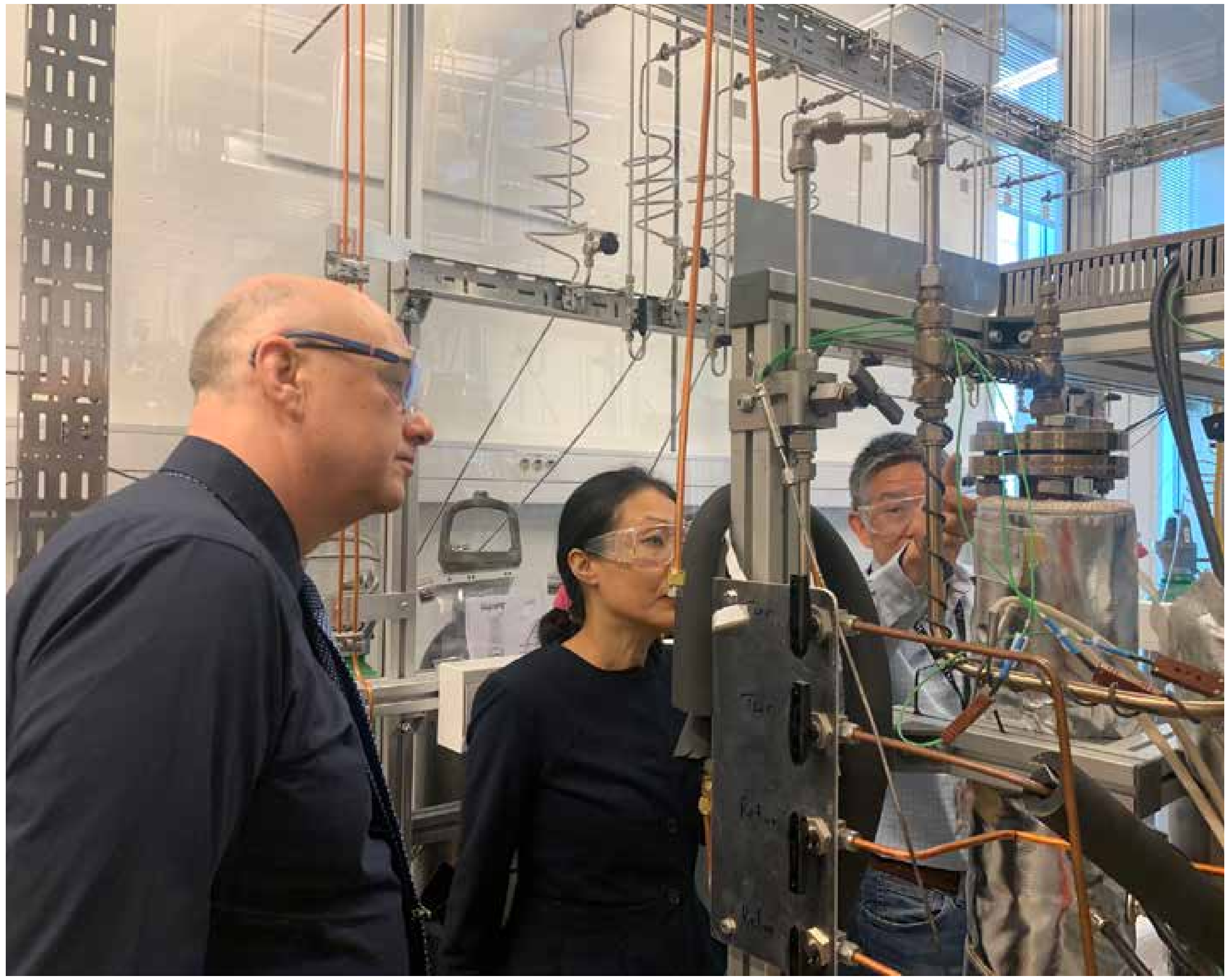
Stable and economic iridium catalysts for renewable energy technologies. UK Catalysis Hub. iCSI-partner involved: NTNU. International partners: Manchester Metropolitan University, UCL, Cardiff University Harwell Research Complex, AVS. Duration: 2021-2023

InnCapPlant – Innovative moving bed adsorption process for CO_2 capture in coal-fired power plants operated under variable load. EØS-Poland. iCSI-partners involved: SINTEF, NTNU. International partners: Cracow University of Technology (CUT). Duration: 2021-2023

Continued membership in the Swiss-Norwegian Beamlines (SNBL) at ESRF. NFR INFRASTRUKTUR. iCSI-partners involved: NTNU, UiO. Other Norwegian partners: IFE, UiB, UiS. Duration: 2021-2024

NoViCo: Novel biorefinery concepts for valorization of lignocellulosic residues, . iCSI-partner involved: SINTEF, International partners: Riga Technical University, The Estonian University of Life Science. Duration: 2021-2024

INTRICat - Analyzing Intermediates of Reactions and Isomers in Catalysis Engineering with Advanced Ion Mass-Spectrometry. iCSI-partner involved: UiO. International partner: University of Oulu Duration: 2021-2024



The INTPART-CATHEX project has given us the opportunity to bring reputable international researchers to Norway for exchange of kowledge and experiences. Here, visiting professors Cathy Chin, University of Toronto and Günther Rupprechter, TU Wien were shown the experimental rigs in the NTNU laboratories.

Accounts 2023

All cost and budget numbers appear in 1000 Norwegian Kroner, kNOK, as of March 2024 NOK 100 are equivalent to € 8,7.

Table 1 summarizes the costs in 2023 and the total budget for the period of the Centre after revision in January 2024.
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 rental of research equipment acquired to serve needs for the SFI
- Other operating expenses includes mainly research at industrial partners

Cost code	Costs 2023	Total costs 2015-2023
Payroll and indirect expenses	7 334	58 826
Procurement of R&D services	11 339	93 074
Equipment	1 380	9 913
Other operating expenses	4 082	34 948
Totals	**24 135**	**196 760**

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	Accounts 2023		Total accounts 2015-2023	
Partner	Costs	Financing	Costs	Financing
NTNU	9 911	3 775	77 184	28 952
University of Oslo	6 436	472	49 462	13 214
SINTEF	4 902		43 611	7 942
Industrial partners	2 885	5 396	26 502	50 502
Research Council of Norway		14 492		96 150
Totals	**24 135**	**24 135**	**196 760**	**196 760**

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 2023	Total costs 2015-2023
IIA1 21st century Nitric Acid technology development	4 645	39 089
IIA2 New NOx abatement technologies	920	8 667
IIA3 Frontier formalin technology development	2 186	24 427
IIA4 PVC Value Chain	3 770	31 869
IIA5 The next step in direct activation of methane	5 267	34 247
IIA6 Generic projects	1 082	34 142
IIA7 2020 Catalysis	3 857	8 195
iCSI Management and administration	2 409	16 125
Totals	**24 135**	**196 760**

Education

Postdoctoral researchers with financial support from iCSI

Sebastian Prodinger	UiO	Austria	2020-2023	M	IIA5
Tina Bergh	NTNU	Norway	2021-2023	F	IIA6
Torstein Fjermestad[1]	UiO	Norway	2022-2024	M	IIA5

1) Granted by iCSI 8 months in 2023

Postdoc Sebastian Prodinger completed his iCSI research in July 2023. He continued at the University of Oslo after being granted NOK 8 million in support from RCN's Researcher Project for Young Talents (FRIPRO) for his project Advanced Synthesis Designs to Unlock Redox/Acidity Cooperativity in Nanoporous Materials for Selective Oxidation Reactions (KeyMAT). Sebastian has decided, however, to continue his career with iCSI partner Topsoe, starting from March 2024. We wish him success in the new job!

Sebastian Prodinger giving a lecture at iCSI's finalising seminar in June.

PhD candidates with financial support from iCSI

Samuel Regli[1]	NTNU	Switzerland	2016-2019	M	IIA6
Moses Mawanga[2]	NTNU	Uganda	2018-2021	M	IIA6
Karoline Kvande[3]	UiO	Norway	2019-2022	F	IIA5
Julie Hessevik[5]	UiO	Norway	2019-2023	F	IIA1
Wei Zhang[4]	NTNU	China	2020-2023	F	IIA4
Jithin Gopakumar[5]	NTNU	India	2020-2024	M	IIA1
Youri van Valen[5]	NTNU	Netherlands	2020-2024	M	IIA3
Bjørn Gading Solemsli[6]	UiO	Norway	2021-2024	M	IIA5
Björn Frederik Baumgarten[5]	NTNU	Germany	2021-2024	M	IIA6

1) Samuel Regli has held a position as lab engineer at IKP, NTNU since August 2020, and his defense is expected to take place in 2024.
2) Moses Mawanga left NTNU for a position in industry 31.12.2022, and his defense is expected to take place in 2024.
3) Karoline Kvande's defense took place 08.08.2023.
4) Wei Zhangs's defense took place 17.11.2023.
5) Julie Hessevik, Jithin Gopakumar, Youri van Valen and Björn Frederik Baumgarten are expected to defend their theses within 2024.
6) Bjørn Gading Solemsli will defend his PhD thesis June 14, 2024

PhD candidates working on projects in iCSI with financial support from other sources

Ole H. Bjørkedal	NTNU	Norway	2016-2020	M	Selective catalytic reduction (SCR) of NO_x emissions in maritime transport.
Martina Cazzolaro	NTNU	Italy	2017-2020	F	Cu/CNF for selective hydrogenation of hydroxyacetone to 1,2-propanediol
Daniel Skodvin	NTNU	Norway	2017-2021	M	Carbon Nanomaterial-Ionic Liquid Hybrid for Ultrahigh Energy Supercapacitor
Jibin Antony	NTNU	India	2018-2022	M	Nanostructured hybrid catalysts for photocatalytic applications
Mario Ernesto Casalegno	NTNU	Mexico	2018-2022	M	Catalyst for onboard hydrogen generation from bioethanol
Ask Lysne	NTNU	Norway	2019-2022	M	Staging and Multiple Hydrogen Feed of Biomass to Fischer-Tropsch Fuel Synthesis
Dumitrita Spinu	NTNU	Romania	2019-2022	F	Low temperature CO_2 capture
Junbo Yu	NTNU	China	2019-2022	M	Hydrogen membrane separation technology
Monica Pazos Urrea [1)]	NTNU	Columbia	2020-2023	F	Kinetic studies of aqueous phase reforming including deactivation studies
Petter Tingelstad	NTNU	Norway	2020-2023	M	Catalytic upgrading of bio-oil to aviation fuels
Oscar Ivanez Encinas	NTNU	Spain	2020-2023	M	Biofuels production from Biomass
Kishore Rajendran	NTNU	India	2020-2023	M	Development of efficient catalyst for conversion of biomass to aviation fuel
Albert Miró i Rovira	NTNU	Spain	2021-2024	M	Catalytic upgrading of bio-oil to aviation fuels
Zhihui Li	NTNU	China	2021-2024	F	Conversion of biomass and plastic wastes
Sahra Louise Guldahl-Ibouder	NTNU	Norway	2023-2026	F	Development of novel materials for low-temperature ammonia cracking
Alicia San Martin Rueda	NTNU	Spain	2023-2026	F	In-situ characterisation of perovskites using advanced techniques
Hammad Ali	NTNU	Pakistan	2023-2026	M	Hydro pyrolysis of plastic waste to produce aviation fuel using ex-situ upgrading catalysts
Mei Ju Goemans	NTNU	The Netherlands	2023-2026	F	Direct conversion of CO_2 and hydrogen to fuels
Erlend Aunan	UiO	Norway	2018-2023	M	Thermochemical Stability and Adsorptive Properties of MOF-808
Martin Myhre Jensen [2)]	UiO,	Norway	2018-2023	M	Pt-Rh nanoparticles for ammonia oxidation
Vladyslav Shostak	UiO	Ukraine	2020-2023	M	Development of comprehensive diffusion/ adsorption models for TAP kinetic experiments
Dag Sannes	UiO	Norway	2020-2023	M	Rational design of MOF catalysts for CO_2 conversion
Mouhammad Abu Rasheed	UiO	Syria	2021-2024	M	Testing of bioinspired catalysts for alkane partial oxidation
Claudia Fabris	UiO	Italy	2022-2025	F	Operando studies of zeolite catalysts
Agnieszka Seremak	UiO	Poland	2022-2025	F	Diffusion, reaction, and entropy in zeolites
Walace Kierulf-Vieira	UiO	Norway	2022-2026	M	Nanoparticles for thermal- and photo catalysis

1) Monica Pazos Urrea defended her PhD thesis 01.12.2023
2) Martin Myhre Jensen defended his PhD thesis 01.03.2024. His work has been a part of WP6.2 in IIA6.

International exchange PhD candidates in iCSI, NTNU

Nikhil Kumar	Indian Institute of Technology Madras	5 months	M	Catalytic Fast Pyrolysis of biomass to produce Fuels and chemicals
Pio Gramazio	University of Bologna	6 months	M	Membrane materials for hydrogen production, Pd based and ceramic membranes
Wiktor Pacura	AGH University	2 weeks	M	
Evangelos Smith	University of Wisconsin Madison	3 months	M	

Postdoctoral researchers working on projects in iCSI with financial support from other sources

Katarzyna Swirk	NTNU	Poland	2020-2023	F	MesoSi-CO_2. Design of low-cost and carbon-resistant Ni-based mesoporous silicas for chemical CO_2 utilization through tri-reforming of methane
Hongfei Ma	NTNU	China	2021-2023	M	Chemical transformation of enzymatic hydrolysis lignin (EHL) with catalytic solvolysis to fuel commodities under mild conditions (EHLCATHOL)
Ainara Moral	NTNU	Spain	2021-2023	F	Moving Bed Carbonate Looping
Felix Herold	NTNU	Germany	2021-2023	M	Carbon materials
Pio Gramazio	NTNU	Italy	2023-2025	M	Direct conversion of CO_2 and hydrogen to fuels
Izar Capel Berdiell	UiO	Spain	2021-2023	M	Catalyst deactivation studies
Abdulla Bin Afif	UiO	India	2023	M	Operando/in-situ Reactor STM and TEM for catalyst development for reactions as ammonia slip and CO_2 utilization

Master's students in Chemical engineering[1] (NTNU) or Chemistry[2] (UiO) in iCSI

Mathilde Ingeborg Nilsen Verne	UiO, iCSI	Norway	2021-2023	F	In-situ XPS of PtRh NPs for NH_3 oxidation
Daniel Levent Arnes	UiO	Norway	2021-2023	M	Methanol-mediated conversion of CO_2 and H_2 to light hydrocarbons
Cathinka S. Carlsen	UiO	Norway	2022-2024	F	Platinum group metal transport in ammonia combustion and recovery
Phillip A. Mørch	UiO	Norway	2022-2024	M	MOF(UiO-66)-Cu(Ni, Au, Pd) nanoparticle hybrid materials for photo- and thermal catalytic conversion of CO_2
Live Bjørnereim Lybekk	UiO	Norway	2022-2024	F	Supported Cu based nanoparticles for thermal- and photo catalysis
Andrea Kjønli	NTNU	Norway	2022-2023	F	Catalytic pyrolysis of waste plastic to liquids
Hammad Ali	NTNU	Pakistan	2022-2023	M	Fast Pyrolysis and upgrading of biomass
Ida Saxrud	NTNU	Norway	2022-2023	F	Catalysts for Syngas Conditioning for Advanced Biofuels
Tomasz Skrzydlo	NTNU, iCSI	Poland	2022-2023	M	Oxidation of methanol to formaldehyde (MTF) over Ag catalyst
Pål Martin Benum	NTNU, iCSI	Norway	2022-2023	M	Catalytic Oxidation of NO to NO_2 at Industrial Nitric Acid Conditions
Sahra Louise Guldahl-Ibouder	NTNU	Norway	2022-2023	F	Model catalysts for fundamental insights into the Fischer-Tropsch Synthesis
Robert Lennard Peters	NTNU	The Nether-lands	2022-2023	M	Ketonisation of acetic acid
Alicia San Martin Rueda	NTNU	Spain	2022-2023	F	Catalysts for advanced biofuels synthesis via the Fischer-Tropsch process
Nora Nyberget Corneliussen	NTNU	Norway	2023-2024	F	Fast pyrolysis of biomass and catalytic upgrading
Jørgen Skjæveland	NTNU	Norway	2023-2024	M	Upscaling of biofuel production by hydrode-oxygenation (HDO) of pyrolysis bio-oil
Sunaina Poonacha Muckatira	NTNU	India	2023-2024	F	Catalytic co-pyrolysis of plastic wastes and biomass to naphtha
Kai Hoang Dinh	NTNU	Norway	2023-2024	M	Integrated pyrolysis and catalytic upgrading of plastic wastes
Andrine Jenssen	NTNU	Norway	2023-2024	F	Direct air capture
Thomas Nhan Nguyen	NTNU	Norway	2023-2024	M	Catalytic purification of pyrolysis oil
Ingrid Johanne Paulsen	NTNU, iCSI	Norway	2023-2024	F	Indium-enhanced Iron catalysts for CO_2 Hydrogenation
Kristin Haukaas Hagen	NTNU, iCSI	Norway	2023-2024	F	Carbon combustion synthesis of a CO_2 to Methanol catalyst
Sander Ose Velle	NTNU	Norway	2023-2024	M	Pd-alloy catalysts and membranes for hydrogen technology
Emma Birkeland	NTNU	Norway	2023-2024	F	Catalytic Steam Reforming of Hydrocarbon Impurities from Biomass Gasification
Rebecka Børresen Anda	NTNU	Norway	2023-2024	F	Mesoporous silicas derived from rice husk for chemical CO_2 utilization

1) Associated with iCSI through specialization project in autumn and master thesis project in spring the second year of the master's studies
2) Associated with iCSI through master's studies over two years

International exchange master's students associated with iCSI

Mei Ju Anne Goemans	Master NTNU	The Nether-lands	5 months	F	Cobalt Catalyzed Fischer-Tropsch-Synthesis: Systematic Studies on Carbon Support Effects on Catalyst Activity and Deactivation
Simon Meilinger	Master NTNU	Germany	2 months	M	Characterisation and Screening of Heteroatom-Doped Carbon Nanofibre Supported Platinum Catalysts for Aqueous Phase Reforming
Matilde Emanuelli	Bachelor NTNU	Italy	3 months	M	Characterization of silver catalysts surface

Master's students from NTNU joined the KinCat (NTNU/SINTEF catalysis group) skiing day in March 2023.

Communication and Dissemination 2023

iCSI Invited Plenaries:

Unni Olsbye: Thermo-catalytic conversion of CO_2 and H_2 to higher hydrocarbons. 9th UK Catalysis Conference; 2023-01-04 - 2023-01-06

Fjermestad, Torstein; Uglietti, Riccardo; Micale, Daniele; Bracconi, Mauro; Phan, Anh; Striolo, Alberto; Iacoviello, Francesco; Svelle, Stian; Maestri, Matteo: Modelling the Methanol to Dimethyl ether reaction – coupling kinetics with transport from CM to Å scale. SMN winter seminar; 2023-01-11 - 2023-01-13

Fjermestad, Torstein; Uglietti, Riccardo; Micale, Daniele; Bracconi, Mauro; Phan, Anh; Striolo, Alberto; Iacoviello, Francesco; Svelle, Stian; Maestri, Matteo: Modelling the Methanol to Dimethyl Ether Reaction – Coupling Kinetics with Transport from CM to Å Scale. Guest lecture, IntriCAT meeting; 2023-01-23 - 2023-01-24

Magnus Rønning: Operando characterisation of catalysts in chemical processes at demanding reaction environments. Guest lecture at research seminar at The Department of Chemical Engineering, University of Manchester; 2023-03-27 - 2023-03-27

Magnus Rønning: Operando characterisation of catalysts in demanding sample environments. LINXS Catalysis Workshop; 2023-05-02 - 2023-05-03

Unni Olsbye: Oxygenate-Mediated Conversion of H_2/CO_x to Hydrocarbons: Influence of Heteroatom and Gas Composition on Zeotype Performance, 28th North American Catalysis Society Meeting, Providence, USA, 2023-06-18 – 2023-06-23

De Chen: Engineering of Catalytic Cycles in Redox Reactions, 15th EuropaCat 2023 Congress, Prague, Czechia, 2023-08-27 - 2023-09-01

Pablo Beato: Catalysis for Sustainable Fuels, 15th EuropaCat 2023 Congress, Prague, Czechia, 2023-08-27 - 2023-09-01Svelle, Stian.

Stian Svelle: Zeolite catalysis research at the University of Oslo. Invited lecture at seminar at TU Eindhoven; 2023-09-07 - 2023-09-07

Popular dissemination

J. Gopakumar, P.M. Benum, I.-H. Svenum, B.C. Enger, D. Waller, M. Rønning: X-ray spectroscopy experiments unravel the transformations of ruthenium catalysts during nitric acid production, ERSF News, Spotlight on science, 2024-02-19

iCSI Publications and conference contributions 2023

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

Journal Publications

Asbjørn Slagtern Fjellvåg, David Waller, Thomas By, and Anja Olafsen Sjåstad: Pt-Catchment Using Pd/Au Alloys: Effect of Enhanced Diffusion, Ind. Eng. Chem. Res. 2023, 62, 6, 2478–2493

Gopakumar, Jithin; Martin Benum, Pål; Svenum, Ingeborg-Helene; Enger, Bjørn Christian; Waller, David; Rønning, Magnus: Redox transformations of Ru catalyst during NO oxidation at industrial nitric acid production conditions. Chemical Engineering Journal 2023, Volume 475, 146406

Gopakumar, Jithin; Vold, Sunniva; Enger, Bjørn Christian; Waller, David; Vullum, Per Erik; Rønning, Magnus: Catalytic oxidation of NO to NO_2 for industrial nitric acid production using Ag-promoted MnO_2/ZrO_2 catalysts. Catalysis Science Technology, 2023, 13, 2783-2793

Holme B., Håkonsen S. F., Waller D.: Challenges in quantifying Pt concentrations in Pd alloys by using secondary ion mass spectrometry: Strong grainorientation effects. Surf Interface Anal. 2024;1-12.

J. Gopakumar, A. Miro i Rovira, B.C. Enger, D. Waller, M. Rønning, Comparison of Ceria-Supported Catalysts for Attaining NO - NO_2 Equilibrium at Industrial Nitric Acid Plant Conditions, 2024 (submitted)

J. Gopakumar, R. Myrstad, R. Børresen Anda, H. Øien, B.C. Enger, D. Waller, M. Rønning, Ostwald Process Intensification by Catalytic Oxidation of Nitric Oxide, 2024 (submitted)

Oral Presentations

Jithin Gopakumar, NTNU: Ruthenium catalysts to attain NO-NO_2 equilibria at Industrial nitric acid conditions, iCSI Annual seminar, Trondheim, Norway, 2023-06-5 – 2023-06-07

Anja O. Sjåstad, David Waller: Main achievements in research and innovation in Industrial Innovation Area 1, iCSI Annual seminar, Trondheim, Norway, 2023-06-5 – 2023-06-07

Anja O. Sjåstad: On the ammonia oxidation reaction, iCSI and CATHEX seminar, Trondheim 2023-06-05-2023-06-08

Posters

Magnus Rønning: Effect of support on Ru-based catalysts in oxidation of nitric oxide for nitric acid production, 15th EuropaCat 2023 Congress, Prague, Czechia, 2023-08-27 - 2023-09-01

IIA2: Abatement of nitrogen-containing pollutants. State-of-the-art catalyst technology

Oral Presentations

Silje F. Håkonsen: Phosphorous contamination of a V/W-TiO_2 Monolith Catalysts used for NH_3-SCR of NOx in bio-fuel combustion exhaust, 15th EuropaCat 2023 Congress, Prague, Czechia, 2023-08-27 - 2023-09-01

Silje F. Håkonsen and Karl Isak Skau: Main achievements in research and innovation in Industrial Innovation Area 2, iCSI Annual seminar, Trondheim, Norway, 2023-06-5 – 2023-06-07

IIA3: Frontier Formalin Technology Development Journal Publications

Oral Presentations

Youri van Valen: Effects of Co-feeding reactants in H_2 and CO oxidation over Silver, iCSI Annual seminar, Trondheim, Norway, 2023-06-5 – 2023-06-07

Jasmina H. Cavka, Ole Bjørkedal Håvik, and Ann Kristin Lagmannsveen: Main achievements in research and innovation in Industrial Innovation Area 3, iCSI Annual seminar, Trondheim, Norway, 2023-06-5 – 2023-06-07

Posters:

Youri van Valen: Oxidation of Methanol to Formaldehyde over Silver Using an Annular Reactor, 15th EuropaCat 2023 Congress, Prague, Czechia, 2023-08-27 - 2023-09-01

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

Journal Publications

Zhang, Wei; Fenes, Endre; Ma, Hongfei; Sollund, Erling Olav; Margossia, Tigran; Rout, Kumar Ranjan; Chen, De: Promoter doping for tuning the redox behavior of $CuCl_2/\gamma\text{-}Al_2O_3$-based catalysts in ethylene oxychlorination: Insights from kinetic studies, Chemical Engineering Journal 2023, Volume 47, 144393

Zhang, Wei; Ma, Hongfei; Wang, Yalan; Rout, Kumar Ranjan; Margossian, Tigran; Chen, De: Toward Fully Selective Ethylene Oxychlorination through Engineering the Cu Oxidation State Spatial Profile, ACS Catalysis 2023, 13, 12, 15107-15114

Hongfei Ma, Xiuhui Zheng, Hao Zhang, Guoyan Ma, Wei Zhang, Zheng Jiang, De Chen: Atomic Cu-N-P-C Active Complex with Integrated Oxidation and Chlorination for Improved Ethylene Oxychlorination, Advanced Science, 2023, Volume 10(8), 2205635

Zhang, Wei; Ma, Hongfei; Wang, Yalan; Regli, Samuel K.; Rønning, Magnus; Rout, Kumar Ranjan; Margossian, Tigran; Chen, De: In situ monitoring of dynamic behavior of La-doped $CuCl_2/\gamma\text{-}Al_2O_3$ catalyst in ethylene oxychlorination. Journal of Catalysis 2023; Volume 417, 314-322

Oral Presentations

De Chen and Dennis Neu Reaction Network and Kinetic Modeling of By-Product Formation in Ethylene Oxychlorination for $CuCl_2/\gamma\text{-}Al_2O_3$-Based Catalysts, 28th North American Catalysis Society Meeting, Providence, USA, 2023-06-18 – 2023-06-23

Wei Zhang, Mechanism and Kinetic Studies of Ethylene Oxychlorination to Ethylene Dichloride and Vinyl Chloride, iCSI Annual seminar, Trondheim, Norway, 2023-06-5 – 2023-06-07

De Chen: Main achievements in research and innovation in Industrial Innovation Area 4, iCSI Annual seminar, Trondheim, Norway, 2023-06-5 – 2023-06-07

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

Journal Publications

Bjørn Gading Solemsli, Izar Capel Berdiell, Sebastian Prodinger, Karoline Kvande, Gabriele Deplano, Unni Olsbye, Pablo Beato, Silvia Bordiga, Stian Svelle: Reactivity of Methoxy species towards Methylation and Oligomerization in Cu-Zeolite systems, Catalysis Today, 2024, submitted.

Karoline Kvande, Beatrice Garetto, Gabriele Deplano, Matteo Signorile, Bjørn Gading Solemsli, Sebastian Prodinger, Unni Olsbye, Pablo Beato, Silvia Bordiga, Stian Svelle, and Elisa Borfecchia: Understanding C-H activation in light alkanes over Cu-MOR zeolites by coupling advanced spectroscopy and temperature-programmed reduction experiments, Chemical Science, 2023, 14, 9704-9723

Karoline Kvande, Moses Mawanga, Sebastian Prodinger, Bjørn Gading Solemsli, Jia Yang, Unni Olsbye, Pablo Beato, Edd Anders Blekkan, and Stian Svelle: Microcalorimetry on Cu-MCM-22 reveals structure-activity relationships for the methane-to-methanol reaction, Industrial Engineering Chemistry Research, 2023, 62 (28), 10939-10950

Karoline Kvande, Sebastian Prodinger, Bjørn Gading Solemsli, Silvia Bordiga, Elisa Borfecchia, Unni Olsbye, Pablo Beato, Stian Svelle: Cu-loaded zeolites enable the selective activation of ethane to ethylene at low temperatures and pressure, Chemical Communications, 2023, 59, 6052-6055

Karoline Kvande, Sebastian Prodinger, Fabian Schlimpen, Pablo Beato, Patrick Pale, Stefan Chassaing, Stian Svelle: Copper-zeolites prepared by solid-state ion exchange - characterization and evaluation for the direct conversion of methane to methanol, Topics in Catalysis, 2023, Volume 66, 1406-1417

Prodinger, Sebastian; Capel Berdiell, Izar; Cordero-Lanzac, Tomás; Reidar Bygdnes, Odd; Solemsli, Bjørn; Kvande, Karoline; Bjørnar Arstad, Beato, Pablo; Olsbye, Unni; Svelle, Stian: Cation-Induced Speciation of port-Size during mordenite zeolite synthesis, Journal of Materials Chemistry A, 2023, 11, 21884-21894

Sun, Xinwei; Vøllestad, Einar; Rørvik, Per Martin; Prodinger, Sebastian; Kalantzopoulos, Georgios; Chatzitakis, Athanasios; Norby, Truls: Surface protonic conductivity in chemisorbed water in porous nanoscopic CeO_2. Applied Surface Science 2023, Volume 611,155590

Oral Presentations

Svelle, Stian; Capel Berdiell, Izar; Wragg, David Stephen; Beato, Pablo; Lundegaard, Lars Fahl: In situ and operando X-ray diffraction as a tool to monitor zeolite catalyst deactivation. Operando VII - the 7th International Congress on Operando Spectroscopy; 2023-05-07 - 2023-05-11

Bjørn Gading Solemsli: Methylation versus oligomerization of light Alkenes and Benzene through stepwise reaction with Methane in Cu-Exchanged Zeolites, iCSI Annual seminar, Trondheim, Norway, 2023-06-5 – 2023-06-07

Stian Svelle: Main achievements in research and innovation in Industrial Innovation Area 5, iCSI Annual seminar, Trondheim, Norway, 2023-06-5 – 2023-06-07

Sebastian Prodinger: Developing Synthesis-Structure-Activity Relationships for the Partial Oxidation of Methane: Achievements and Outlook, iCSI Annual seminar, Trondheim, Norway, 2023-06-5 – 2023-06-07

B. G. Solemsli, S. Prodinger, K. Kvande, G. Deplano, U. Olsbye, S. Bordiga, P. Beato, S. Svelle: Methylation of light alkenes and aromatics though step-wise reaction with methane in Cu-exchanged Zeolites, 15th EuropaCat 2023 Congress, Prague, Czechia, 2023-08-27 - 2023-09-01

Posters

Sebastian Prodinger: Cation-induced Speciation of Port-Size in MOR Zeolite Synthesis, 15th EuropaCat 2023 Congress, Prague, Czechia, 2023-08-27 - 2023-09-01

IIA6: Generic Projects for Additional Industrial Synergies

Journal Publications

Ingeborg-Helene Svenum, Marie D. Strømsheim, Jan Knudsen, Hilde J. Venvik: Activity and segregation behavior of $Pd_{75\%}Ag_{25\%}$(111) during CO oxidation – An in-situ NAP-XPS investigation, Journal of Catalysis, 2023, Volume 417, 194-201

Thronsen, Elisabeth; Bergh, Tina; Thorsen, Tor Inge; Christiansen, Emil; Frafjord, Jonas; Crout, Philip; Van Helvoort, Antonius Theodorus Johannes; Midgley, Paul A.; Holmestad, Randi: Scanning precession electron diffraction data analysis approaches for phase mapping of precipitates in aluminium alloys. Ultramicroscopy 2024, Volume 255, 113861

Bergh, Tina; Fyhn, Hursanay; Sandnes, Lise; Blindheim, Jørgen; Grong, Øystein; Holmestad, Randi; Berto, Filippo; Vullum, Per Erik: Multi-material Joining of an Aluminum Alloy to Copper, Steel, and Titanium by Hybrid Metal Extrusion & Bonding. Metallurgical and Materials Transactions A 2023, Volume 54, 2689-2702

Jensen, Martin Myhre; Kierulf-Vieira, Walace; Kooyman, Patricia J.; Sjåstad, Anja Olafsen: Variable temperature in situ TEM mapping of the thermodynamically stable element distribution in bimetallic Pt–Rh nanoparticles. Nanoscale Advances 2023, Volume 5, 5286-529

Mehdi Mahmoodinia, Hammad Farooq, Torbjørn Røe, Ingeborg-Helene Svenum, Hilde J. Venvik: Effect of Copper Catalyst Content and Zinc Promoter on Carbon Formation in the Direct Synthesis of Methylchlorosilanes, Ind. Eng. Chem. Res. 2023, Volume 62 (50), 21579–21589 4

Moses Mawanga, Jia Yang and Edd Anders Blekkan, Steady-State and Transient Kinetic Investigations of the Oxidation of NO over Pt/SiO_2, Journal of Catalysis, 2024, submitted.

Oral Presentations

Thronsen, Elisabeth; Bergh, Tina; Thorsen, Tor Inge; Christiansen, Emil; Frafjord, Jonas; Crout, Philip; Van Helvoort, Antonius Theodorus Johannes; Midgley, Paul Anthony; Holmestad, Randi: Phase mapping of precipitates in Al alloys by 4D-STEM. INTPART workshop; 2023-04-14 - 2023-04-15

Bjørn Baumgarten: Reducing coking by coupling CO_2 Hydrogenation and MTO, , iCSI and CATHEX seminar, Trondheim, Norway, 2023-06-5 – 2023-06-08

Magnus Rønning: Main achievements in research and innovation in Industrial Innovation Area 6, iCSI Annual seminar, Trondheim, Norway, 2023-06-5 – 2023-06-07

Magnus Rønning: Lessions learned from operando characterisation of catalysts in demanding sample environments, iCSI and CATHEX seminar, Trondheim, Norway, 2023-06-5 – 2023-06-08

Bergh, Tina; Venvik, Hilde Johnsen: Developing electron microscopy and diffraction methods for catalyst characterisation at NTNU. iCSI and CATHEX Seminar; Trondheim 2023-06-05 - 2023-06-08

Svenum, Ingeborg-Helene; Strømsheim, Marie D.; Knudsen, Jan; Mahmoodinia, Mehdi; Shavorskiy, Andrey; Yu, Junbo; Boix, Virgínia; Peters, Thijs; Venvik, Hilde Johnsen: In situ NAP-XPS characterization of PdAg single crystals and polycrystalline thin films, 15th EuropaCat 2023 Congress, Prague, Czechia, 2023-08-27 - 2023-09-01

Posters

Svenum, Ingeborg-Helene; Strømsheim, Marie Døvre; knudsen, Jan; Venvik, Hilde Johnsen: Surface reactivity and segregation dynamics of Pd-Ag alloy surfaces by NAP-XPS. Reactions at Surface Active Sites: From Single Atoms and 2D Materials to Electrified Interfaces; 2023-02-12 - 2023-02-17

Svenum, Ingeborg-Helene; Strømsheim, Marie Døvre; Shavorskiy, Andrey; Yu, Junbo; Peters, Thijs; Venvik, Hilde Johnsen: Surface reactivity and segregation dynamics of Pd-Ag alloy surfaces by NAP-XPS. Chemical Reactions at Surfaces GRC: Reactions at Surface Active Sites: From Single Atoms and 2D Materials to Electrified Interfaces; 2023-02-12 - 2023-02-17

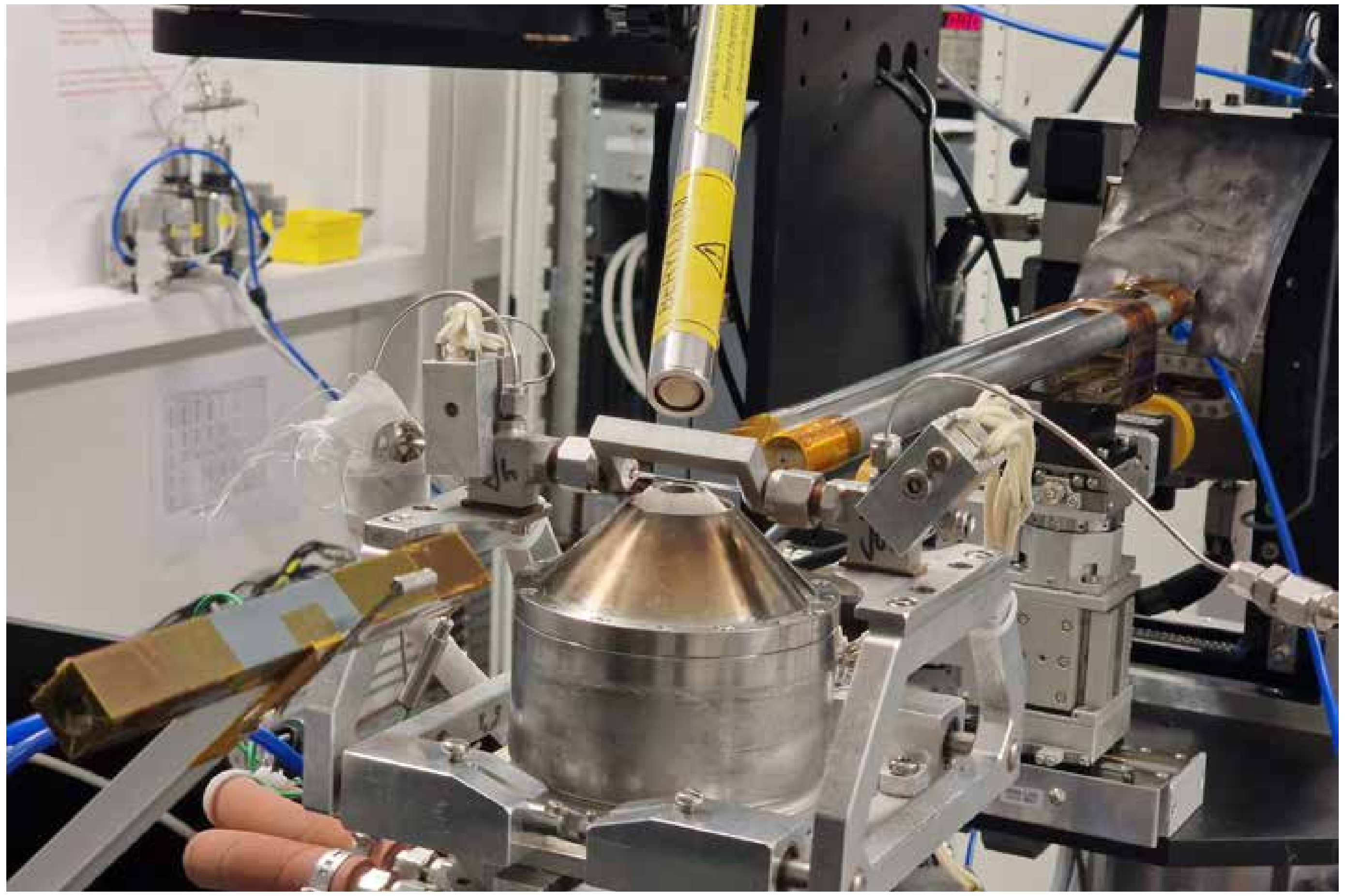


Photo: Magnus Rønning

Björn Frederik Baumgarten: Particle size effect for CO_2 hydrogenation by In_2O_3-ZrO_2 catalysts, 15th EuropaCat 2023 Congress, Prague, Czechia, 2023-08-27 - 2023-09-01

Tina Bergh: Three-dimensional electron microscopy characterisation of silver before and after oxidation of CO, H_2 and CH_3OH, 15th EuropaCat 2023 Congress, Prague, Czechia, 2023-08-27 - 2023-09-01

iCSI Associated Journal Publications

Antony, Jibin; Villa Gonzalez, Susana; Bandyopadhyay, Sulalit; Yang, Jia; Rønning, Magnus: Silica-modified bismutite nanoparticles for enhanced adsorption and faster solar photocatalytic degradation of methylene blue. Catalysis Today, 2023, Volumes 413–415, 113986

Banu S, Lathifa; Veerapandy, Vasu; Fjellvåg, Helmer; Ponniah, Vajeeston: First-Principles Insights into the Relative Stability and Physical and Chemical Properties of $MoSe_2$, ACS Omega, 2023, Volum 8 (15), 13799-13812

C. Rosmini, M. Pazos Urrea, E. Tusini, S. Indris, D. Kovacheva, D. Karashanova, H. Kolev, A. Zimina, J.-D. Grunwald, M. Rønning, M. Dimitrov, M. Popov: Unveiling the synergistic effects of pH and Sn content for tuning the catalytic performance of $Ni0/Ni_xSn_y$ intermetallic compounds dispersed on Ce-Zr mixed oxides in the aqueous phase reforming of ethylene glycol, App. Cat. B, 2024, 350, 123904

Capa, A.; González-Vázquez, M.P.; Chen, De; Rubiera, F.; Pevida, C.; Gil, M.V.: Effect of H_2S on biogas sorption enhanced steam reforming using a Pd/Ni-Co catalyst and dolomite as a sorbent. Chemical Engineering Journal 2023, Volume 476, 146803

Capel Berdiell, Izar; Braghin, Giorgio Bruno; Cordero-Lanzac, Tomas; Beato, Pablo; Lundegaard, Lars F.; Wragg, David Stephen; Bordiga, Silvia; Svelle, Stian: Tracking Structural Deactivation of H-Ferrierite Zeolite Catalyst During MTH with XRD, Topics in catalysis, 2023, Volume 66, 1418–1426

Choudhary, Mukesh K.; Fjellvåg, Helmer; Ponniah, Ravindran: First principle studies on electronic and thermoelectric properties of Fe_2TiSn based multinary Heusler alloys. Computational Materials Science, 2023, Volume 216, 111856

Cordero-Lanzac, Tomas; Ramirez, Adrian; Cruz-Fernandez, Marta; Zander, Hans-Jörg; Joensen, Finn; Woolas, Steven; Meiswinkel, Andreas; Styring, Peter; Gascon, Jorge; Olsbye, Unni: A CO_2 valorization plant to produce light hydrocarbons : Kinetic model, process design and life cycle assessment. Journal of CO_2 Utilization, 2023, Volume 67, 102337-

Chen, Wenyao; Zuo, Ji; Sang, Keng; Qian, Gang; Zhang, Jing; Chen, De; Zhou, Xinggui; Yuan, Weikang; Duan, Xuezhi: Leveraging the Proximity and Distribution of Cu–Cs Sites for Direct Conversion of Methanol to Esters/Aldehydes. Angewandte Chemie International Edition 2024, Volume 63 (1), e202314288

Cheng, Gong; Wang, Xin-Xin; Zhang, Shuai-Hui; Zhu, Ka-Ke; Sui, Zhi-Jun; Zhou, Xing-Gui; Chen, De; Zhu, Yi-An: On the product and transition-state shape selectivities in 2-heptene isomerization. Chemical Physics Letters 2023, Volume 812, ID 140263

Fan, Guifang; Chen, De; Li, Shizhong; Yang, Mingde; Wu, Yulong: Effect of Metal Oxides on Reaction Route and Product Distribution of Catalytic Cellulose Hydrogenolysis. BioResources, 2023, Volume 18 (4), 7367-7390

Farooq, Muhammad U.; Shi, Yao; Chen, Wenyao; Guan, Yanan; Zhou, Jinghong; Song, Nan; Qian, Gang; Zhang, Jing; Chen, De; Zhou, Xinggui; Duan, Xuezhi: Kinetics insights into the active sites of Au catalysts for the oxidative esterification of methacrolein to methyl methacrylate. Chemical Engineering Science (CES), 2023, Volume 277, 118840

Fei, Zhaofu; Chen, De; Hensen, Emiel J.M.; Li, Yongdan; Jagadeesh, Rajenahally V.: Catalytic valorization of lignocellulose and its derived feedstocks into fuels and chemicals. Catalysis Today 2023, Volume 408, 1

Feng, Xiang; Hu, Han; Chen, De: Key nanomaterials for industrial chemical process. Nano Reseach, 2023, Volume 16, 6013–6014

Hayoune, Asma; Akkari, Hocine; Marelli, Marcello; Pappalardo, Valeria; Yang, Jia; Zubair, Muhammad: Synthesis and characterization of iron sulfide immobilized on Algerian halloysite clay (HKDD3) with enhanced removal of methylene blue from aqueous medium. Surface and Interface Analysis, 2024, Volume 56 (1), 52-61

Hempel, Frida Sveen; Martineau-Corcos, Charlotte; Bianchini, Federico; Fjellvåg, Helmer; Arstad, Bjørnar: Dynamics of Interlayer Na-Ions in Ga-Substituted $Na_2Zn_2TeO_6$ (NZTO) Studied by Variable-Temperature Solid-State ^{23}Na NMR Spectroscopy and DFT Modeling, ACS Physical Chemistry Au, 2023, 3, 4, 394–405

Herold, Felix; Imhof, Timo; Roumeliotis, Paul; Schühle, Patrick; Ledendecker, Marc; Rønning, Magnus: Controlled doping of carbon catalyst supports by atomic replacement via gasification-assisted heteroatom doping. Carbon 2023, Volume 207, 207-218

Ivanez Encinas, Oscar Luis; Groven, Anette Synnøve; Rout, Kumar Ranjan; Blekkan, Edd Anders: Phosphorus deactivation on co-based catalysts for Fischer-Tropsch. Topics in catalysis 2023, Volume 66, 1381-1390

Jing, Li-Jun; Yan, Wei-Qi; Xiao, Han-Jie; Lei, Ming; Cao, Yue-Qiang; Sui, Zhi-Jun; Zhou, Jing-Hong; Zhou, Xing-Gui; Chen, De; Zhu, Yi-An: Interface-enhanced catalytic performance of TiO_2 supported Cu and Au for dimethyl oxalate hydrogenation: A comparative microkinetic analysis. Chemical Engineering Science (CES), , Volume 281, 119176

Li, Ruiying; Zheng, Xiuhui; Wang, Fei; Yan, Hao; Zhou, Xin; Tuo, Yongxiao; Liu, Yibin; Feng, Xiang; Chen, Xiaobo; Chen, De; Yang, Chaohe: Optimizing Mo-C coordination for enhanced low-temperature water-gas shift activity over α-MoC_{1-x} catalysts: An experimental and theoretical study. Chemical Engineering Journal 2023, Volume 474, 145645

Lin, Dong; Feng, Xiang; Zheng, Xiuhui; Xu, Yang; Zhao, Hui; Song, Zhaoning; Wang, Liang; Shan, Honghong; Xiao, Feng-Shou; Chen, De; Yang, Chaohe: Dimensional Regulation of Titanosilicate by Kinetically Controlled Intergrowth Crystals. Advanced Functional Materials 2023, Volume33 (23), 2301179

Lin, Dong; Mao, Zhiwei; Feng, Xiang; Zhou, Xin; Yan, Hao; Zhu, Huihong; Liu, Yibin; Chen, Xiaobo; Tuo, Yongxiao; Peng, Chong; Chen, De; Yang, Chaohe: Kinetic insights into deoxygenation of vegetable oils to produce second-generation biodiesel. Fuel 2023, Volume 333 (2), 126416

Lundegaard, Lars Fahl; Capel Berdiell, Izar; König, Nico; Junge, Nicolai Haaber; Beato, Pablo; Chernyshov, Dmitry; Svelle, Stian; Wragg, David Stephen: Tracking deactivation of zeolite beta with and without a detailed structure model: XRD analysis and in situ studies, Microporous and Mesoporous Materials, 2023, Volum 366, 112911

M. Pazos Urrea, S. Meilinger, F. Herold, J. Gopakumar, E. Tusini, A. De Giacinto, A. Zimina, J.-D. Grunwald, D. Chen, M. Rønning: Aqueous phase reforming on carbon-doped supported metal catalysts: Exploring platinum-heteroatom interactions, ACS Catal., 2024, 14, 4139–4154

Ma, Guoyan; Wang, Le; Wang, Xiaorong; Wang, Chengjun; Li, Xi; Li, Lu; Chen, De: Preparation and Properties of Poly(vinyl acetate) Adhesive Modified with Vinyl Versatate. Molecules 2023, Volume 28 (18), 6634

Ma, Jianyu; Mahmoodinia, Mehdi; Rout, Kumar Ranjan; Blekkan, Edd Anders: High-temperature sulfur capture by a Mn-Mo sorbent: An investigation of regeneration conditions and SO_2 formation and prevention. Chemical Engineering Science (CES) 2023, Volume 274, 118674

Meng, Fanyu; Yan, Hao; Zhou, Xiaoqing; Zeng, Jie; Zhou, Xin; Liu, Yibin; Feng, Xiang; Chen, De; Yang, Chaohe: Carbon-based metal-free catalysts for selective oxidation of glycerol to glycolic acid. Chemical Engineering Science (CES), 2023, Volume 268, 118394

Muthukrishnan, S.; Vidya, R.; Sjåstad, Anja Olafsen: Band gap engineering of anatase TiO_2 by ambipolar doping: A first principles study. Materials Chemistry and Physics, 2023, Volume 299, 127467

Pazos Urrea, Monica; Herold, Felix; Chen, de; Rønning, Magnus: Nitrogen-containing carbon nanofibers as supports for bimetallic Pt-Mn catalysts in aqueous phase reforming of ethylene glycol. Catalysis Today 2023, Volume 418, 114066

Pulumati, Sri Harsha; Sannes, Dag Kristian; Jabbour, Christia R.; Mandemaker, Laurens D. B.; Weckhuysen, Bert M.; Olsbye, Unni; Nova Flores, Ainara; Skúlason, Egill: Mechanistic Insights in the Catalytic Hydrogenation of CO_2 over Pt Nanoparticles in UiO-67 Metal-Organic Frameworks. ACS Catalysis, 2023, Volume 14 (1), 382-394

Redekop, Evgeniy; Cordero-Lanzac, Tomás; Salusso, Davide; Pokle, Anuj; Øien-Ødegaard, Sigurd; Sunding, Martin Fleissner; Diplas, Spyridon; Negri, Chiara; Borfecchia, Elisa; Bordiga, Silvia; Olsbye, Unni: Zn Redistribution and Volatility in $ZnZrO_x$ Catalysts for CO_2 Hydrogenation. Chemistry of Materials, 2023, Volume 35 (24), 10434-10445

Sannes, Dag Kristian; Øien-Ødegaard, Sigurd; Aunan, Erlend; Nova, Ainara; Olsbye, Unni: Quantification of Linker Defects in UiO-Type Metal-Organic Frameworks. Chemistry of Materials, 2023, Volume 35 (10), 3793-3800

Song, Zhaoning; Yan, Hao; Yuan, Juncong; Ma, Hongfei; Cao, Jianlin; Wang, Yongxiang; Wang, Qiang; Peng, Chong; Deng, Feng; Feng, Xiang; Chen, De; Yang, Chaohe; Hu, Yongkang: Engineering a Coordinatively Unsaturated Au–O–Ti^{3+} Structure Toward Unprecedented H_2 Efficiency for Low-Temperature Propene Epoxidation with H_2 and O_2. Engineering (Beijing), 2023, Volume 25 (6), 144-156

Summa, Paulina; Swirk, Katarzyna; Gopakumar, Jithin; Samojeden, Bogdan; Motak, Monika; Rønning, Magnus; Van Beek, Wouter; Da Costa, Patrick: Optimization of Co-Ni-Mg-Al mixed-oxides CO_2 methanation catalysts with solution combustion synthesis: On the importance of Co incorporation and basicity. Applied Materials Today, 2023, Volume 32, 101795

Sun, Zongzhuang; Zhou, Xin; Song, Zhaoning; Yan, Hao; Tuo, Yongxiao; Liu, Yibin; Zhao, Hui; Chen, Xiaobo; Feng, Xiang; Chen, De; Yang, Chaohe: Numerical calculation of flow and reaction safety with different particle sizes in a fixed bed reactor for propene epoxidation with H_2 and O_2. Chemical Engineering Science (CES), 2023, Volume 277, 118777

Świrk Da Costa, Katarzyna; Summa, Paulina; Gopakumar, Jithin; van Valen, Youri; Da Costa, Patrick; Rønning, Magnus: Excess-Methane CO_2 Reforming over Reduced KIT-6-Ni-Y Mesoporous Silicas Monitored by In Situ XAS–XRD. Energy & Fuels, 2023, 37, 23, 18952–18967

Tezel, Elif; Sannes, Dag Kristian; Svelle, Stian; Szilagyi, Petra Agota; Olsbye, Unni: Direct CO_2 to methanol reduction on Zr_6-MOF based composite catalysts: A critical review, Materials Advances, 2023, 4, 5479-5495

Ticali, Pierfrancesco; Salusso, Davide; Airi, Alessia; Morandi, Sara; Borfecchia, Elisa; Ramirez, Adrian; Cordero-Lanzac, Tomas; Gascon, Jorge; Olsbye, Unni; Joensen, Finn; Bordiga, Silvia: From Lab to Technical CO_2 Hydrogenation Catalysts: Understanding PdZn Decomposition. ACS Applied Materials & Interfaces, 2023, Volume 15(4), 5218-5228

Tuo, Yongxiao; Liu, Wanli; Lu, Qing; Wang, Xingzhao; Luo, Jiabing; Wang, Shutao; Zhou, Yan; Wang, Min; Sun, Xiaohui; Feng, Xiang; Wu, Mingbo; Chen, De; Zhang, Jun: SO_4^{2-} mediated CO_2 activation on metal electrode for efficient CO_2 electroreduction. Chemical Engineering Journal, 2023, Volume 464, 142510

Tuo, Yongxiao; Lu, Qing; Liu, Wanli; Wang, Min; Zhou, Yan; Feng, Xiang; Wu, Mingbo; Chen, De; Zhang, Jun: Atomic Zn-Doping Induced Sabatier Optimum in $NiZn_{0.03}$ Catalyst for CO_2. Electroreduction at Industrial-Level Current Densities, Small, 2023, Early version2306945

Tuo, Yongxiao; Meng, Ying; Lu, Qing; Wang, Qing; Jia, Furong; Zhou, Yan; Feng, Xiang; Zhang, Jun; Duan, Xuezhi; Chen, De: Taming Pt 5d state occupancy via Pt-O-Mn electronic linkage for enhanced dehydrogenation activity. AIChE Journal, 2023, Volume 69.(9), e18149

Xie, Jingxiu; Olsbye, Unni: The Oxygenate-Mediated Conversion of CO_x to Hydrocarbons – On the Role of Zeolites in Tandem Catalysis, Chemical Reviews, 2023, Volume 123 (20), 11775-11816

Yan, Hao; Liu, Bowen; Zhou, Xin; Meng, Fanyu; Zhao, Mingyue; Pan, Yue; Li, Jie; Wu, Yining; Zhao, Hui; Liu, Yibin; Chen, Xiaobo; Li, Lina; Feng, Xiang; Chen, De; Shan, Honghong; Yang, Chaohe; Yan, Ning: Enhancing polyol/sugar cascade oxidation to formic acid with defect rich MnO_2 catalysts. Nature Communications, 2023, Volume 14 (1), 4509

Zhao, Guanghui; Deng, Xuliang; Lin, Dong; Liu, Jincheng; Zhang, Yong-Jun; Liu, Yibin; Chen, Xiaobo; Feng, Xiang; Chen, De; Yang, Chaohe; Shan, Honghong: Constructing Highly Efficient Ti Sites of TS-1 for Alkene Epoxidation, Industrial & Engineering Chemistry Research, 2023, 62, 44, 18205–18229

Zhou, Xin; Li, Zhiyang; Feng, Xiang; Yan, Hao; Chen, De; Yang, Chaohe: A hybrid deep learning framework driven by data and reaction mechanism for predicting sustainable glycolic acid production performance. AIChE Journal, 2023, Volume 69 (7), e18083

iCSI Associated Oral Presentations

Brennhagen, Anders; Cavallo, Carmen; Wragg, David Stephen; Koposov, Alexey; Ponniah, Vajeeston; Sjåstad, Anja Olafsen; Fjellvåg, Helmer: Tracing the (De)sodiation of Bi_2MoO_6 Through Good and Bad Times With Operando XRD. NKS-FUM 2023; 2023-02-13 - 2023-02-14

Ainara Moral Larrasoana: Dechlorination of plastic waste derived pyrolysis oil, iCSI and CATHEX seminar, Trondheim 2023-06-05-2023-06-08

Albert Miro í Rovira: Hydrodeoxygenation of bio-oil, iCSI and CATHEX seminar, Trondheim 2023-06-05-2023-06-08

Ask lysne: Hydrotalcite-Derived Nickel-Cobalt Catalysts for Steam Reforming of Bio-Syngas Hydrocarbon Impurities, iCSI and CATHEX seminar, Trondheim 2023-06-05-2023-06-08

Felix Herold: Controlled Doping of Carbon Catalyst Supports by Atomic Replacement via Gasification-Assisted Heteroatom Doping, iCSI and CATHEX seminar, Trondheim 2023-06-05-2023-06-08

Jia Yang: Iron based Fischer Tropsch synthesis, iCSI and CATHEX seminar, Trondheim 2023-06-05-2023-06-08

Monica Pazos Urrea: Utilizing carbon nanofiber-supported catalysts for hydrogen production via aqueous phase reforming of ethylene glycol, iCSI and CATHEX seminar, Trondheim 2023-06-05-2023-06-08

Oscar Luis Ivanez Encinas: Poisoning of cobalt based catalysts in FT, iCSI and CATHEX seminar, Trondheim 2023-06-05-2023-06-08

Tomas Cordero-Lanzac, Adiran Ramirez, Marta Cruz-Fernandez, Hans-Jörg Zander, Finn Joensen, Andreas Meiswinkel, Jorge Gascon and Unni Olsbye: Kinetic Model, Process Design and LCA of a CO_2 Valorization Plant to Produce Light Hydrocarbon Using a Pdzn/ZrO_2 + SAPO-34 Catalyst, 28th North American Catalysis Society Meeting, Providence, USA, 2023-06-18 – 2023-06-23

PhD candidate from Veronica Piazza from Politecnico de Milano, who had a guest stay at NTNU in 2022, disussing with candidates from NTNU catalysis group at the EuropaCat 2023 poster session.

Ainara Moral: Understanding of Fe reduction in the dechlorination of plastic waste derived pyrolysis oil using chlorobenzene as model compound, 15th EuropaCat 2023 Congress, Prague, Czechia, 2023-08-27 - 2023-09-01

Bjørn Gading Solemsli: Methylation of light alkenes and aromatics though step-wise reaction with methane in Cu-exchanged Zeolites, 15th EuropaCat 2023 Congress, Prague, Czechia, 2023-08-27 - 2023-09-01

Ingeborg-Helene Svenum: Understanding the interaction of CH_3Cl with Cu-based surfaces, 15th EuropaCat 2023 Congress, Prague, Czechia, 2023-08-27 - 2023-09-01

Oscar Ivanez Encinas: Phosphorus deactivation of cobalt-based catalysts for Fischer-Tropsch Synthesis, 15th EuropaCat 2023 Congress, Prague, Czechia, 2023-08-27 - 2023-09-01

Pazos Urrea, Monica; Herold, Felix; Meilinger, Simon; Gopakumar, Jithin; Tusini, Enrico; De Giacinto, Andrea; Zimina, Anna; Chen, de; Grunwaldt, Jan-Dierk; Rønning, Magnus: Aqueous-phase reforming of ethylene glycol over platinum-based catalysts supported on functionalised carbon nanofibres, 15th EuropaCat 2023 Congress, Prague, Czechia, 2023-08-27 - 2023-09-01

Petter Tingelstad: Vapour phase upgrading of acetic acid over noble metal promoted metal oxides at hydropyrolysis conditions: reaction mechanisms and pathways, 15th EuropaCat 2023 Congress, Prague, Czechia, 2023-08-27 - 2023-09-01

Torstein Fjermestad: Modelling the methanol to dimethyl ether reaction – coupling kinetic with transport from Å to cm scale, 15th EuropaCat 2023 Congress, Prague, Czechia, 2023-08-27 - 2023-09-01

iCSI Associated Posters

Agnieszka Seremak: Theoretical study of local and global deformation of H-ZSM-5, 15th EuropaCat 2023 Congress, Prague, Czechia, 2023-08-27 - 2023-09-01

Albert Miró i Rovira: Hydrodeoxygenation of anisole over Pd/TiO2 catalyst: pressure-dependent reaction pathways, 15th EuropaCat 2023 Congress, Prague, Czechia, 2023-08-27 - 2023-09-01

Ask Lysne: Steam Reforming of Bio-Syngas Hydrocarbon Impurities with Ni-Co/Mg(Al)O Catalysts – Operating Parameter Effects, 15th EuropaCat 2023 Congress, Prague, Czechia, 2023-08-27 - 2023-09-01

Brennhagen, Anders; Skautvedt, Casper; Cavallo, Carmen; Skurtveit, Amalie; Wragg, David Stephen; Koposov, Alexey; Vajeeston, Ponniah; Sjåstad, Anja Olafsen; Fjellvåg, Helmer: Revealing the Cycling and Degradation Mechanism of Bi-Metallates as Anode Materials fro Na-ion Batteries. 244th ECS Meeting; 2023-10-08 - 2023-10-12

Capel Berdiell, Izar; Wragg, David Stephen; Beato, Pablo; Lundegaard, Lars Fahl; Di Michel, Marco; Svelle, Stian: Temperature Programmed Oxidation Probed with X-ray Diffraction Computed Tomography, 15th EuropaCat 2023 Congress, Prague, Czechia, 2023-08-27 - 2023-09-01

Kishore Rajendran: Two-step configuration of carbon-carbon coupling and hydrodeoxygenation catalyst for the upgradation of biomass derived oxygenates, 15th EuropaCat 2023 Congress, Prague, Czechia, 2023-08-27 - 2023-09-01

Petra Agota Szilagyi: Pd nanoclusters confined in functionalised metal-organic frameworks: selective, active and stable catalysts for hydrogenation reactions, 15th EuropaCat 2023 Congress, Prague, Czechia, 2023-08-27 - 2023-09-01

Rama, Raquel J.; Nova, Ainara; Olsbye, Unni: Synthesis of linker-based bifunctional ligands for UiO-67 metal-organic frameworks. 6th EuChemS Inorganic Chemistry Conference; 2023-09-03 - 2023-09-074.

Sannes, Dag Kristian; Øien-Ødegaard, Sigurd; Aunan, Erlend; Nova Flores, Ainara; Olsbye, Unni: Quantification of linker defects in UiO-type metal-organic frameworks. EUROMOF 2023; 2023-09-23 - 2023-09-27

Svelle, Stian; Capel Berdiell, Izar; Wragg, David Stephen; Beato, Pablo; Lundegaard, Lars Fahl: In situ and operando X-ray diffraction as a tool to monitor zeolite catalyst deactivation. Operando VII The 7th International Congress on Operando Spectroscopy; 2023-05-07 - 2023-05-11

Unni Olsbye: Copper-catalyzed peroxidation of cyclohexane in liquid phase: an elucidation of mechanism and cycle stability of Cu(I) and Cu(II) in tetradentate N,N,N,N-Cu complexes, 15th EuropaCat 2023 Congress, Prague, Czechia, 2023-08-27 - 2023-09-01

Zhihui Li: Co-pyrolysis of biomass and plastic to produce high-quality liquid, 15th EuropaCat 2023 Congress, Prague, Czechia, 2023-08-27 - 2023-09-01

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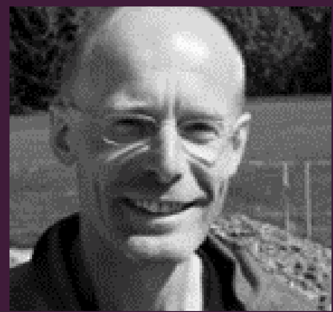

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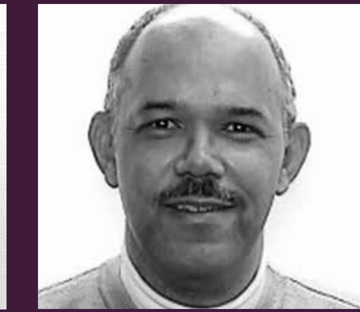

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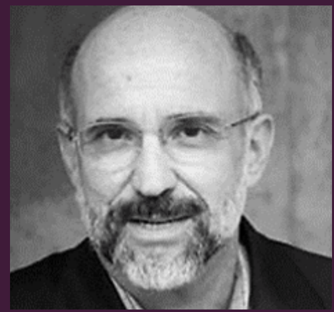

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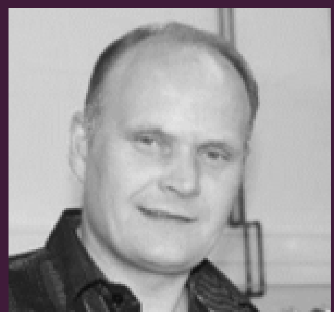
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Acknowledgements

The authors acknowledge all the contributors to the Annual Report 2023:

Stian Svelle, UiO and Jithin Gopakumar, NTNU for Scientific Highlights. Summaries of Scientific activities are by Silje Fosse Håkonsen, SINTEF; Youri van Valen, NTNU; De Chen, NTNU; Stian Svelle, UiO; Anja Olafsen Sjåstad, UiO; Björn Frederik Baumgarten, NTNU. The authors thank Semantix for proofreading. The professional photographers Thor Nielsen, Hilde Skar Olsen, Benjamin A. Ward have photos on page 7, 12 and 33, respectively. In addition, we are grateful that many from the iCSI community have shared photos from their iCSI Moments 2023. Last but not least, thanks to Marianne Gilbu at the NTNU Grafisk Senter for her efforts in making the report presentable.

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