Photocatalysis of methane using non-noble metal oxides

Trial lecture

Karoline Kvande
University of Oslo, Department of Chemistry. SMN
11.08.2023
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 sabatical 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.

Educing 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!
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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.

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 Inovyn and Haldor Topsoe 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.

INOVYN

INEOS Inovyn Ltd. is a leading producer of chlorovinyls 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 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.

KA RASMUSSEN

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.

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 iCSIs internationalization and recognition.

Management and Administration

The Centre is hosted by the Department of Chemical Engineering at NTNU. The administration team consists of a Centre Director, a Coordinator/Vice Director (50 % position) and an Economy Advisor (20 % position).
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.

“When 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.

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?

“From the tasks 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 have 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.

“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.”

“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 new-born 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.”

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 Renning 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.

In 1994, it was not common for women with children inside or outside of their belly to get doctorates. Adresseavisen 1994
Scientific Highlights 2023: Collaboration is the path to success

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 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 NH3 and CH4 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.

Publications

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); Ivar Capel Berdell (ICSI Postdoc); Pablo Beato (senior scientist at Haldor Topsoe A/S); Bjørn Gading Solemsl (ICSI PhD candidate)
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 NO2 using a series of heat exchangers, and finally, NO2 absorption in water to produce nitric acid. Catalysing the nitric oxide, one of the main steps in the chemical process gas.

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.

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-Al2O3-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 O2 and NO2 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 O2 and NO2 in a 20-minute time frame.

The results reveal the mechanism behind NO oxidation at industrial nitric acid production conditions over γ-Al2O3-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 2  a) In-situ XANES profiles of γ-Al2O3-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 O2 and NO2 during 20 minutes of a total of 3 hours NO oxidation.

Publications

iCSI moments 2023

- Skiing day in March
- Grenoble in July
- The red sweater team
- Engineers have fun
- Daily life in Chemistry building 5
- New PhDs: Wei, Karoline and Monica
Hilde invited to a sushi dinner during the seminar in June

Hyfer seminar in September

Europacat 2023, In Prague in August

Project meetings with Dynea and KAR
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 Iglesias 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.
Program for the iCSI/CATHEX seminar in Trondheim June 5-8 2023.

### Day 1  
**Monday June 5 iCSI seminar, Room R9, NTNU**

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<th>Topic</th>
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<tr>
<td>12:00-13:00</td>
<td>Lunch@Realfagskantina</td>
<td>Main achievements in research and innovation</td>
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<tr>
<td>13:00-13:15</td>
<td>Pablo Beato, Topscie, Chair of the iCSI Board</td>
<td>Welcome to seminar</td>
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<tr>
<td>13:15-13:40</td>
<td>SAS: Anja O. Sjåstad, UIO and David Waller, Yara</td>
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<td>13:40-14:00</td>
<td>SAS: Sijie F. Håkonsen, SINTEF and Karl Isak Skau, Yara</td>
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<td>14:00-14:25</td>
<td>SAS: Jasmina H. Cavka, SINTEF, Ole Bjerkedal Håvik, Dynna and Ann Krystin Lagnmannveen, K. A. Rasmussen</td>
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<td>14:25-14:45</td>
<td>Coffee break</td>
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<td>14:45-15:10</td>
<td>SAS: De Chen, NTNU</td>
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<tr>
<td>15:10-15:25</td>
<td>SAS: Stan Svelle, Univ. of Oslo</td>
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<tr>
<td>15:25-16:00</td>
<td>SAS: Magnus Rennings, NTNU</td>
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<tr>
<td>16-22</td>
<td>Casual dining @Hilde’s garden in Sleipnes vei 5</td>
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### Day 2  
**Tuesday June 6 iCSI seminar, guest from CATHEX are welcome to join, Room R9, NTNU**

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<th>Time</th>
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<tr>
<td>09:00-09:10</td>
<td>Edd Bleekan, NTNU</td>
<td>Welcome</td>
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<tr>
<td>09:10-09:30</td>
<td>Jithin Gopakumar, NTNU</td>
<td>Ruthenium catalysts to attain NO-NO2 equilibria at Industrial nitric acid conditions</td>
</tr>
<tr>
<td>09:30-09:50</td>
<td>Wei Zhang, NTNU</td>
<td>Mechanism and Kinetic Studies of Ethylene Oxychlorination to Ethylene Dichloride and Vinyl Chloride</td>
</tr>
<tr>
<td>09:50-10:05</td>
<td>Youri van Valen, NTNUuw</td>
<td>Effects of Co-feeding reactants in H2 and CO oxidation over Silver</td>
</tr>
<tr>
<td>10:05-10:20</td>
<td></td>
<td></td>
</tr>
<tr>
<td>10:20-10:50</td>
<td></td>
<td></td>
</tr>
<tr>
<td>10:50-11:10</td>
<td>Bjørn Gading Solemsj, Univ. of Oslo</td>
<td>Methylation versus oligomerization of light Alkenes and Benzene through stepwise reaction with Methane in Cu-Exchanged Zeolites.</td>
</tr>
<tr>
<td>11:10-11:25</td>
<td>Dimitrios Pappas, CoorsTek</td>
<td>Experiences after ICSI</td>
</tr>
<tr>
<td>11:25-11:40</td>
<td>Aase Marie Hundere, RCN</td>
<td>Words from the Research Council of Norway</td>
</tr>
<tr>
<td>11:40-11:55</td>
<td>Øyvind Weiby Gregersen, NTNU</td>
<td>Words from Dean of NV faculty</td>
</tr>
<tr>
<td>12:00-13:00</td>
<td>Lunch@Realfagskantina</td>
<td></td>
</tr>
<tr>
<td>13:00-13:30</td>
<td>Hilde J. Venkv, ICSI director</td>
<td>ICSI experiences and achievements</td>
</tr>
<tr>
<td>13:30-14:20</td>
<td>Prof. Enrique Iglesa, Univ. of California, Berkeley, ICSI scientific advisor</td>
<td>Uncovering active sites and reaction channels in C-H activation reactions on oxide catalysts</td>
</tr>
<tr>
<td>14:20-14:40</td>
<td>Coffee break</td>
<td></td>
</tr>
<tr>
<td>14:40-15:30</td>
<td>Prof. Alessandra Beretta, Politecnico di Milano, ICSI scientific advisor</td>
<td>NH3 catalytic cracking: kinetic investigation over Ru-supported catalysts and reactor study with thermally and electrically conductive structured internals</td>
</tr>
<tr>
<td>15:30-15:40</td>
<td>Short break</td>
<td></td>
</tr>
<tr>
<td>15:40-15:55</td>
<td>Bjørn Christian Enger, SINTEF</td>
<td>Catalysis needs for the future (Outlook to 2030)</td>
</tr>
<tr>
<td>15:55-16:00</td>
<td>Pablo Beato, Topscie</td>
<td>Concluding remarks</td>
</tr>
<tr>
<td>16:00-16:30</td>
<td>Break</td>
<td></td>
</tr>
<tr>
<td>16:30-17:30</td>
<td>All</td>
<td>iCSI &amp; CATHEX Poster session</td>
</tr>
<tr>
<td>19-24</td>
<td>Cslation dinner@NINA-kantina</td>
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</table>

### Day 3  
**Wednesday June 7 CATHEX/icsi seminar, Room R9, NTNU**

<table>
<thead>
<tr>
<th>Time</th>
<th>Who</th>
<th>Topic</th>
</tr>
</thead>
<tbody>
<tr>
<td>09:00-09:10</td>
<td>Ingeborg-Helene Svenum, NTNU</td>
<td>Welcome</td>
</tr>
<tr>
<td>09:10-09:50</td>
<td>Ya Yang, Shanghai Jiao Tong Univ.</td>
<td>Iron based Fischer Tropsch synthesis</td>
</tr>
<tr>
<td>09:50-10:30</td>
<td>Manos Marvinkakis, Univ. of Wisconsin-Madison</td>
<td>Challenging well-established assumptions for the active site in heterogeneous catalysis</td>
</tr>
<tr>
<td>10:30-11:00</td>
<td>Coffee break</td>
<td></td>
</tr>
<tr>
<td>11:00-11:20</td>
<td>Tina Bergh, iCSI@NTNU</td>
<td>Developing transmission electron microscopy methods for catalyst characterisation at NTNU</td>
</tr>
<tr>
<td>11:20-12:00</td>
<td>Cathy Chin, Univ. of Toronto</td>
<td>Catalytic Transformation of Light Alkanol and Alkanol Feedstock</td>
</tr>
<tr>
<td>12:00-13:00</td>
<td>Lunch@Realfagskantina</td>
<td></td>
</tr>
<tr>
<td>13:00-13:40</td>
<td>Patricia Kooyman, Univ. of Cape Town</td>
<td>Removal of CO from H2</td>
</tr>
<tr>
<td>13:40-14:20</td>
<td>Anja O. Sjåstad, Univ. of Oslo</td>
<td>On the ammonia oxidation reaction</td>
</tr>
<tr>
<td>14:20-14:40</td>
<td>Coffee break</td>
<td></td>
</tr>
<tr>
<td>14:40-15:20</td>
<td>Michael Claey, Univ. of Cape Town</td>
<td>Direct CO2 hydrogenation for the production of sustainable fuels and chemicals</td>
</tr>
<tr>
<td>15:20-15:40</td>
<td>Huong Lan Haynh, Best Catalysis PhD, Norwegian Chemical Society</td>
<td>CO2 methanation on Ni-Fe based catalysts: mechanistic and structured reactor study</td>
</tr>
<tr>
<td>15:40-16:00</td>
<td>Sebastian Prodinger, iCSI@UIO</td>
<td>Developing Synthesis-Structure-Activity Relationships for the Partial Oxidation of Methane: Achievements and Outlook</td>
</tr>
<tr>
<td>16:00-16:30</td>
<td>Break</td>
<td></td>
</tr>
<tr>
<td>16:30-17:30</td>
<td>All</td>
<td>iCSI &amp; CATHEX Poster session</td>
</tr>
</tbody>
</table>

### Day 4  
**Thursday June 8, CATHEX young researchers day, seniors are welcome to join, Room R9**

<table>
<thead>
<tr>
<th>Time</th>
<th>Who</th>
<th>Topic</th>
</tr>
</thead>
<tbody>
<tr>
<td>09:00-09:10</td>
<td>Petter Tingelstad, NTNU</td>
<td>Welcome</td>
</tr>
<tr>
<td>09:10-09:40</td>
<td>Prof. Magnus Rennings, NTNU</td>
<td>Lessons learned from operando characterisation of catalysts in demanding sample environments</td>
</tr>
<tr>
<td>09:40-09:50</td>
<td>Ask Iysner, NTNU</td>
<td>Hydroxidite-Derived Nickel-Cobalt Catalysts for Steam Reforming of Bio-Syngas Hydrocarbon Impurities</td>
</tr>
<tr>
<td>09:50-10:00</td>
<td>Oscar Luis Iambez Encinas, NTNU</td>
<td>Poisoning of cobalt based catalysts in FT</td>
</tr>
<tr>
<td>10:00-10:10</td>
<td>Thulani Nyath, Univ. of Cape Town</td>
<td>Manganese-cobalt oxide ([MnxCo1-x]3O4) catalysts studied in situ during the preferential oxidation of carbon monoxide</td>
</tr>
<tr>
<td>10:10-10:20</td>
<td>Bjørn Baumgarten, NTNU</td>
<td>Reducing cooking by coupling CD2 Hydrogenation and MTO</td>
</tr>
<tr>
<td>10:20-10:40</td>
<td>Coffee break with discussions</td>
<td></td>
</tr>
<tr>
<td>10:40-10:50</td>
<td>Ainaara Moral Larrassana, NTNU</td>
<td>Dechlorination of plastic waste derived pyrolys oil</td>
</tr>
<tr>
<td>10:50-11:10</td>
<td>Guangming Cai, Univ. of Toronto</td>
<td>Consequences of Site Correlations and Structural Dynamics on Metal Oxides (C-O Formation) (C-H Scission)</td>
</tr>
<tr>
<td>11:10-11:30</td>
<td>William Broomhead, Univ. of Toronto</td>
<td>Catalytic Significance of the Oxide-Support Interface in Alkanol Oxidative Dehydrogenation</td>
</tr>
<tr>
<td>11:30-11:50</td>
<td>Coffee break with discussions</td>
<td></td>
</tr>
<tr>
<td>11:50-12:00</td>
<td>Felix Herold, NTNU</td>
<td>Controlled Doping of Carbon Catalyst Supports by Atomic Replacement via Gasification-Assisted Heteroatom Doping</td>
</tr>
<tr>
<td>12:00-12:10</td>
<td>Evangelos Smith, Univ. of Wisconsin-Madison</td>
<td>Reactive liquid crystals for the design of chemoresponsive hydrogen sensors</td>
</tr>
<tr>
<td>12:10-12:20</td>
<td>Monica Pazos Urrea, NTNU</td>
<td>Utilizing carbon nanofiber-supported catalysts for hydrogen production via aqueous phase reforming of ethylene glycol</td>
</tr>
<tr>
<td>12:20-12:30</td>
<td>Albert Miro i Rivira, NTNU</td>
<td>Hydrodeoxygenation of bio-oil</td>
</tr>
<tr>
<td>12:30-13:00</td>
<td>Lunch</td>
<td></td>
</tr>
<tr>
<td>13:30</td>
<td>Social activities (optional )</td>
<td></td>
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</table>

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**Anniversary Report 2023 - ICSI - 26**

**26 - ICSI - Annual Report 2023**

**Annual Report 2023 - ICSI - 27**
Scientific Activities
Scientific Activities

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

**IIA1**
21st Century Ammonia Oxidation and Nitric Acid technology development

**IIA2**
New NOx abatement technologies for the marine market and state-of-the-art SCR catalysis

**IIA3**
Frontier formalin technology development

**IIA4**
PVC Value Chain: World class energy and raw material efficiency for the production of Chlorine and Vinyl Chloride Monomer (VCM)

**IIA5**
The next step in direct activation of lower alkanes

**IIA6**
Generic projects for additional industrial synergies

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

The IIA1 team 2023

<table>
<thead>
<tr>
<th>Role</th>
<th>Name</th>
<th>Institute</th>
</tr>
</thead>
<tbody>
<tr>
<td>IIA leader, PhD supervisor and WP responsible (WP1.1), advisor (WP1.2)</td>
<td>Anja Olafsen Sjåstad</td>
<td>UiO</td>
</tr>
<tr>
<td>Advisor (WP1.1-1.2)</td>
<td>Helmer Fjellvåg</td>
<td>UiO</td>
</tr>
<tr>
<td>PhD candidate (WP1.1)</td>
<td>Julie Hessevik</td>
<td>UiO</td>
</tr>
<tr>
<td>Researcher (WP 1.1)</td>
<td>Martin Jensen</td>
<td>UiO</td>
</tr>
<tr>
<td>Researcher (WP 1.1)</td>
<td>Henrik Sætesby</td>
<td>UiO</td>
</tr>
<tr>
<td>Master’s student (WP1.1)</td>
<td>Cathinka S. Carlsen</td>
<td>UiO</td>
</tr>
<tr>
<td>Industry senior researcher (WP1.1-1.2-1.3), PhD supervisor (WP1.1)</td>
<td>David Waller</td>
<td>YARA</td>
</tr>
<tr>
<td>Industry researcher (WP 1.1)</td>
<td>Daniela Farmer</td>
<td>YARA</td>
</tr>
<tr>
<td>Industry researcher (WP 1.1)</td>
<td>Oskar Iveland</td>
<td>YARA</td>
</tr>
<tr>
<td>Industry researcher (WP 1.1)</td>
<td>Marianne S. Granvold</td>
<td>YARA</td>
</tr>
<tr>
<td>Industry researcher (WP 1.1)</td>
<td>Torgeir Lunde</td>
<td>YARA</td>
</tr>
<tr>
<td>Industry researcher (WP 1.1)</td>
<td>Ann Kristin Lagmannsveen</td>
<td>KA Rasmussen</td>
</tr>
<tr>
<td>Industry researcher (WP 1.1-1.2)</td>
<td>Federica Mudu</td>
<td>KA Rasmussen</td>
</tr>
<tr>
<td>Researcher WP responsible (WP1.2)</td>
<td>Sille Fosse Håkonsen</td>
<td>SINTEF</td>
</tr>
<tr>
<td>Researcher (WP 1.2)</td>
<td>Børge Holme</td>
<td>SINTEF</td>
</tr>
<tr>
<td>Researcher (WP 1.2)</td>
<td>Martin F. Sunding</td>
<td>SINTEF</td>
</tr>
<tr>
<td>Senior Engineer (WP1.2)</td>
<td>Kari Anne Brendefal</td>
<td>SINTEF</td>
</tr>
<tr>
<td>Research engineer (WP1.2)</td>
<td>Joanna Pierchala</td>
<td>SINTEF</td>
</tr>
<tr>
<td>PhD supervisor, WP responsible (WP1.3)</td>
<td>Magnus Rønning</td>
<td>NTNU</td>
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<tr>
<td>PhD candidate (WP1.3)</td>
<td>Jithin Gopakumar</td>
<td>NTNU</td>
</tr>
<tr>
<td>Master’s student (WP1.3)</td>
<td>Pål Martin Benum</td>
<td>NTNU</td>
</tr>
<tr>
<td>PhD supervisor, senior researcher (WP1.3)</td>
<td>Rune Lødeng</td>
<td>SINTEF</td>
</tr>
<tr>
<td>Senior researcher (WP1.3)</td>
<td>Bjørn Christian Enger</td>
<td>SINTEF</td>
</tr>
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</table>

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 PtO2(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 NH3 over 10 days on stream causes heavy reconstruction. Cross-sections of wires from selected experiments are shown in Figure 1. The images clearly show that when either NO or NH3 was present, the original dense Pd wires have...
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% O2 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 O2 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 O2 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 O2, 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.

Publication
Publications and conference contributions from IIA1 in 2023 are listed on page 58.
Motivation
When ammonia is combusted in a nitric acid plant in the Oswald process to produce NOx, N2O is an unwanted by-product. The levels of N2O might appear to be low but the high Global Warming Potential (GWP) of N2O 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 Co and Al spinel phase supported on CeO2. This catalyst can achieve > 95% abatement with no changes to plant operation. The deN2O 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 deN2O 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 CoAl2O4, while a green colour indicates the spinel phase Co2AlO4. 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-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.
IIA3: Frontier Formalin Technology Development

The IIA3 team 2023

<table>
<thead>
<tr>
<th>Name</th>
<th>Institution</th>
<th>Role</th>
</tr>
</thead>
<tbody>
<tr>
<td>Jasmina Hafizovic Cavka</td>
<td>SINTEF</td>
<td>IIA leader</td>
</tr>
<tr>
<td>Hilde Venvik</td>
<td>NTNU</td>
<td>PhD supervisor, WP responsible</td>
</tr>
<tr>
<td>Jia Yang</td>
<td>NTNU</td>
<td>PhD co-supervisor, advisor</td>
</tr>
<tr>
<td>Youji van Valen</td>
<td>NTNU</td>
<td>PhD candidate</td>
</tr>
<tr>
<td>Matilde Emanuelli</td>
<td>NTNU</td>
<td>Exchange bachelor’s student</td>
</tr>
<tr>
<td>Tina Bergh</td>
<td>NTNU</td>
<td>Postdoctoral fellow</td>
</tr>
<tr>
<td>Tomasz Skrzydlo</td>
<td>NTNU</td>
<td>Master’s student</td>
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<tr>
<td>Ann Kristin Lagnannsveen</td>
<td>KA Rasmussen</td>
<td>Industry researcher</td>
</tr>
<tr>
<td>Federica Mudu</td>
<td>KA Rasmussen</td>
<td>Industry researcher</td>
</tr>
<tr>
<td>Ole H. Bækjedal</td>
<td>DYNAPA</td>
<td>Industry researcher</td>
</tr>
<tr>
<td>Lars Axelsen</td>
<td>SINTEF</td>
<td>PhD co-supervisor, senior researcher</td>
</tr>
<tr>
<td>Rune Ladeng</td>
<td>SINTEF</td>
<td>Senior researcher</td>
</tr>
<tr>
<td>Roman Tschentscher</td>
<td>SINTEF</td>
<td>Senior engineer</td>
</tr>
<tr>
<td>Kari Anne Andreassen</td>
<td>SINTEF</td>
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</table>

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$_3$OH) 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 thin slices (here 30-50 nm thick), before the SEM is employed to image the freshly polished surfaces, as shown in Figure 1. Figure 1a) shows a top-view secondary electron (SE) SEM image of an annular silver catalyst after oxidation of syngas 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 method 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 (STEM) 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.

Publication

Conference contributions from IIA3 are listed on page 59.
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. Granvold  INEOS Inovyn  Industry researcher (WP4.2-4.5)
Andrea Mansella  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 CuCl2/Al2O3 catalyst

This study investigates the promoter effects of 14 metal chlorides (NaCl, KCl, RbCl, CsCl, MgCl2, CaCl2, SrCl2, CeCl3, PrCl3, NdCl3, ErCl3, TmCl3, YCl3, and SnCl2) on the CuCl2/Al2O3-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 CuCl2/Al2O3-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 CuCl2 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 CuCl2/Al2O3-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 CuCl2/Al2O3-based catalysts at a wide conversion range and reveal the importance of spatially distributed CuCl2 concentration for the catalytic performance through the spatial-time resolved UV-Vis-NIR approach. A high CuCl2 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 CuCl2 with specific promoters. Our engineered, tri-promoter doped KMGa-LaCuCl2/Al2O3 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.

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 CuCl2/Al2O3-based catalysts at 220−260°C and low pressure (1−5 bar). 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 C2H4 forming C2H3Cl* (EDC*). The adsorbed EDC* prefers to undergo the dehydrochlorination reaction to VCM* and HCP*, 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 (WPs.1-5.2-5.3)
Unni Olsbye UiO PhD supervisor (WPs.1-5.2)
Karoline Kvande UiO PhD candidate (WPs.1-5.2)
Sebastian Prodingger UiO Postdoctoral fellow (WPs.1-5.2-5.3)
Bjørn Gading Solemsli UiO PhD candidate (WPs.1-5.2)
Izar Capel Berdiell UiO Researcher (WPs.1-5.2)
Torstein Fjermestad UiO Postdoctoral fellow (WPs.1-5.2)
Pablo Beato Haldor Topsøe A/S Industry senior and researcher (WPs.1-5.2-5.3)
Lars Fahl Lundegaard Haldor Topsøe A/S Industry researcher (WPs.1-5.2-5.3)
Søren Birck Rasmussen Haldor Topsøe A/S Industry senior researcher (WPs.1-5.2-5.3)
Aino Nielsen Haldor Topsøe A/S Industry researcher (WPs.1-5.2-5.3)
Mette Christensen Nielsen Haldor Topsøe A/S Industry researcher (WPs.1-5.2-5.3)
Hanne Zin glowing Strumann Haldor Topsøe A/S Industry researcher (WPs.1-5.2-5.3)
Bjørnar Arstad SINTEF Senior researcher (WPs.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, ChemCatChem, 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/H2O, 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. Furthermore, reactions with benzene reveal that only a fraction of the methoxy species are available to react with benzene, and that Bronsted 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.
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 Einger 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-supervisor (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)
Bjorn 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 (NH₃) oxidation for NH₃-slip in the maritime sector (diesel engines and the upcoming NH₃ engines). In the development of stable catalytic bimetallic Pt-Rh nanoparticles, full control of the Pt-Rh alloying and 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 synthesis. 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.

In-situ TEM element mapping

![In-situ TEM element mapping](image)

**Pt-Rh elemental mixing / segregation versus temperature and nanoparticle size**

![Pt-Rh elemental mixing / segregation versus temperature and nanoparticle size](image)
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 GHSV-s between 500 and 5000 ml/gcatmin.

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

$$\Delta m = K_0 \left( \frac{1}{f^2} - \frac{1}{f_0^2} \right)$$

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.
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.

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

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 collaboration 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 (Huoquan), 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
- Ecole Polytechnique Fédérale de Lausanne, Switzerland
- ETH Zurich, Switzerland
- Ghent University, Belgium
- Institut de Recherches sur la Catalyse et l’Environnement de Lyon, CNRS, France
- Instituto Nacional del Carbón, INCAR-CSIC, Spain
- Karlruhe 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 Scherrer Institut, Switzerland
- Politecnico 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?)
- Firmsenich, Switzerland
- ICI Caldaie, Italy
- ILS, Integrated Lab Solutions, Germany
- Johnson Matthey, United Kingdom
- Linde, Germany
- Neste, Finland
- NextChem SP, Italy
- OMV, Austria
- Process design center B.V. (PDC), Netherlands
- Ranida, Czech Republic
- Repsol SA, Spain
- Siemens Energy, Sweden
- Steeper, Denmark
- Tata Steel UK Limited, UK
- Topsoe AS, Denmark
- Total Energies, France
- Turkije Petrol Rafinerileri Anonim Sirketi ( Tupras), Turkey
- UOP LLC, USA
- VTT, Finland
European research - Horizon 2020 and Horizon Europe project


PyroCO2 - Demonstrating sustainable value creation from industrial CO2 by its thermophilic microbial conversion into acetone. LC-GD-3-1-2020. iCSI-partner involved: SINTEF. Duration: 2021-2026.


C4H 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.


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.


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


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.


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.


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


International collaborations supported by RCN and sources other than EU


TOMOCAT - Tracking the deactivation of shaped zeolite catalysts in time and space using X-ray diffraction tomography. iCSI-partner involved: UiO. International partners: Topasoe, University of Turin. Duration: 2020-2024.

The INTPART-CATHEX project has given us the opportunity to bring reputable international researchers to Norway for exchange of knowledge and experiences. Here, visiting professors Cathy Chin, University of Toronto and Günther Rupprecht, 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

<table>
<thead>
<tr>
<th>Cost code</th>
<th>Costs 2023</th>
<th>Total costs 2015-2023</th>
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<tbody>
<tr>
<td>Payroll and indirect expenses</td>
<td>7 334</td>
<td>58 826</td>
</tr>
<tr>
<td>Procurement of R&amp;D services</td>
<td>11 339</td>
<td>93 074</td>
</tr>
<tr>
<td>Equipment</td>
<td>1 380</td>
<td>9 913</td>
</tr>
<tr>
<td>Other operating expenses</td>
<td>4 082</td>
<td>34 948</td>
</tr>
<tr>
<td>Totals</td>
<td>24 135</td>
<td>196 760</td>
</tr>
</tbody>
</table>

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

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

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).

<table>
<thead>
<tr>
<th>Industrial Innovation Area (IIA)</th>
<th>Costs 2023</th>
<th>Total costs 2015-2023</th>
</tr>
</thead>
<tbody>
<tr>
<td>IIA1 21st century Nitric Acid technology development</td>
<td>4 645</td>
<td>39 089</td>
</tr>
<tr>
<td>IIA2 New NOx abatement technologies</td>
<td>920</td>
<td>8 667</td>
</tr>
<tr>
<td>IIA3 Frontier formalin technology development</td>
<td>2 186</td>
<td>24 427</td>
</tr>
<tr>
<td>IIA4 PVC Value Chain</td>
<td>3 770</td>
<td>31 869</td>
</tr>
<tr>
<td>IIA5 The next step in direct activation of methane</td>
<td>5 267</td>
<td>34 247</td>
</tr>
<tr>
<td>IIA6 Generic projects</td>
<td>1 082</td>
<td>34 142</td>
</tr>
<tr>
<td>IIA7 2020 Catalyst</td>
<td>3 857</td>
<td>8 195</td>
</tr>
<tr>
<td>ICSI Management and administration</td>
<td>2 409</td>
<td>16 125</td>
</tr>
<tr>
<td>Totals</td>
<td>24 135</td>
<td>196 760</td>
</tr>
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Education

Postdoctoral researchers with financial support from ICSI

<table>
<thead>
<tr>
<th>Sebastian Prodinger</th>
<th>UiO</th>
<th>Austria</th>
<th>2020-2023</th>
<th>M</th>
<th>IIAS</th>
</tr>
</thead>
<tbody>
<tr>
<td>Tina Bergh</td>
<td>NTNU</td>
<td>Norway</td>
<td>2021-2023</td>
<td>F</td>
<td>IIAS</td>
</tr>
<tr>
<td>Torstein Fjermestad</td>
<td>UiO</td>
<td>Norway</td>
<td>2022-2024</td>
<td>M</td>
<td>IIAS</td>
</tr>
</tbody>
</table>

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 Research 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!

PhD candidates with financial support from ICSI

| Samuel Regli 1)  | NTNU | Switzerland | 2016-2019 | M | IIAS |
| Moses Mawanga 2) | NTNU | Uganda      | 2018-2021 | M | IIAS |
| Karoline Kvande 3) | UiO | Norway      | 2019-2022 | F | IIAS |
| Julie Hessev 4)  | UiO | Norway      | 2019-2023 | F | IIAS |
| Wei Zhang 5)     | NTNU | China       | 2020-2023 | F | IIAS |
| Jithin Gopakumar 6) | NTNU | India       | 2020-2024 | M | IIAS |
| Youri van Valen 7) | NTNU | Netherlands | 2020-2024 | M | IIAS |
| Bjørn Gading Solemsli 8) | UiO | Norway      | 2021-2024 | M | IIAS |
| Bjørn Frederik Baumgarten 9) | NTNU | Germany     | 2021-2024 | M | IIAS |

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.
5) Julie Hessev, Jithin Gopakumar, Youri van Valen and Bjørn 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

<table>
<thead>
<tr>
<th>Name</th>
<th>Institution / Country</th>
<th>Year(s)</th>
<th>Type</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ole H. Bjerkedal</td>
<td>NTNU Norway</td>
<td>2016-2020</td>
<td>M</td>
<td>Selective catalytic reduction (SCR) of NO(_x) emissions in maritime transport.</td>
</tr>
<tr>
<td>Martina Cazzolaro</td>
<td>NTNU Italy</td>
<td>2017-2020</td>
<td>F</td>
<td>Cu/CNF for selective hydrogenation of hydroxyacetone to 1,2-propanediol.</td>
</tr>
<tr>
<td>Daniel Skodvin</td>
<td>NTNU Norway</td>
<td>2017-2021</td>
<td>M</td>
<td>Carbon Nanomaterial-Ionic Liquid Hybrid for Ultra-high Energy Supercapacitor</td>
</tr>
<tr>
<td>Jibin Antony</td>
<td>NTNU India</td>
<td>2018-2022</td>
<td>M</td>
<td>Nanostructured hybrid catalysts for photocatalytic applications</td>
</tr>
<tr>
<td>Mario Ernesto Casaliegno</td>
<td>NTNU Mexico</td>
<td>2018-2022</td>
<td>M</td>
<td>Catalyst for onboard hydrogen generation from bioethanol.</td>
</tr>
<tr>
<td>Ask Lysne</td>
<td>NTNU Norway</td>
<td>2019-2022</td>
<td>M</td>
<td>Staging and Multiple Hydrogen Feed of Biomass to Fischer-Tropsch Fuel Synthesis</td>
</tr>
<tr>
<td>Dumitrita Spinu</td>
<td>NTNU Romania</td>
<td>2019-2022</td>
<td>F</td>
<td>Low temperature CO(_2) capture</td>
</tr>
<tr>
<td>Junbo Yu</td>
<td>NTNU China</td>
<td>2019-2022</td>
<td>M</td>
<td>Hydrogen membrane separation technology</td>
</tr>
<tr>
<td>Monica Pazos Urrea</td>
<td>NTNU Columbia</td>
<td>2020-2023</td>
<td>F</td>
<td>Kinetic studies of aqueous phase reforming including deactivation studies</td>
</tr>
<tr>
<td>Petter Tingestad</td>
<td>NTNU Norway</td>
<td>2020-2023</td>
<td>M</td>
<td>Catalytic upgrading of bio-oil to aviation fuels</td>
</tr>
<tr>
<td>Oscar Ivanez Encinas</td>
<td>NTNU Spain</td>
<td>2020-2023</td>
<td>M</td>
<td>Biofuels production from Biomass</td>
</tr>
<tr>
<td>Kishore Rajendran</td>
<td>NTNU India</td>
<td>2020-2023</td>
<td>M</td>
<td>Development of efficient catalyst for conversion of biomass to aviation fuel</td>
</tr>
<tr>
<td>Albert Miró i Revira</td>
<td>NTNU Spain</td>
<td>2021-2024</td>
<td>M</td>
<td>Catalytic upgrading of bio-oil to aviation fuels</td>
</tr>
<tr>
<td>Zhifeng Li</td>
<td>NTNU China</td>
<td>2021-2024</td>
<td>F</td>
<td>Conversion of biomass and plastic wastes</td>
</tr>
<tr>
<td>Sahra Louise Gulddahl-Ibouter</td>
<td>NTNU Norway</td>
<td>2023-2026</td>
<td>F</td>
<td>Development of novel materials for low-temperature ammonia cracking</td>
</tr>
<tr>
<td>Alicia San Martin Rueda</td>
<td>NTNU Spain</td>
<td>2023-2026</td>
<td>F</td>
<td>In-situ characterisation of perovskites using advanced techniques</td>
</tr>
<tr>
<td>Hammad Ali</td>
<td>NTNU Pakistan</td>
<td>2023-2026</td>
<td>M</td>
<td>Hydro pyrolysis of plastic waste to produce aviation fuel using ex-situ upgrading catalysts</td>
</tr>
<tr>
<td>Mei Ju Goemans</td>
<td>NTNU The Netherlands</td>
<td>2023-2026</td>
<td>F</td>
<td>Direct conversion of CO(_2) and hydrogen to fuels</td>
</tr>
<tr>
<td>Erland Aunan</td>
<td>UiO Norway</td>
<td>2018-2023</td>
<td>M</td>
<td>Thermochemical Stability and Adsorptive Properties of MOF-808</td>
</tr>
<tr>
<td>Martin Myhre Jensen</td>
<td>UiO Norway</td>
<td>2018-2023</td>
<td>M</td>
<td>Pt-Rh nanoparticles for ammonia oxidation</td>
</tr>
<tr>
<td>Vladyslav Shostak</td>
<td>UiO Ukraine</td>
<td>2020-2023</td>
<td>M</td>
<td>Development of comprehensive diffusion/adsorption models for TAP kinetic experiments</td>
</tr>
<tr>
<td>Dag Sannes</td>
<td>UiO Norway</td>
<td>2020-2023</td>
<td>M</td>
<td>Rational design of MOF catalysts for CO(_2) conversion</td>
</tr>
<tr>
<td>Mouhammad Abu Rasheed</td>
<td>UiO Syria</td>
<td>2021-2024</td>
<td>M</td>
<td>Testing of bioinspired catalysts for alkane partial oxidation</td>
</tr>
<tr>
<td>Claudia Fabris</td>
<td>UiO Italy</td>
<td>2022-2025</td>
<td>F</td>
<td>Operando studies of zeolite catalysts</td>
</tr>
<tr>
<td>Agnieszka Seremak</td>
<td>UiO Poland</td>
<td>2022-2025</td>
<td>F</td>
<td>Diffusion, reaction, and entropy in zeolites</td>
</tr>
<tr>
<td>Walace Kierulf-Vieira</td>
<td>UiO Norway</td>
<td>2022-2026</td>
<td>M</td>
<td>Nanoparticles for thermal- and photo catalysis</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>Name</th>
<th>Institution / Country</th>
<th>Year(s)</th>
<th>Type</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nikhil Kumar</td>
<td>Indian Institute of Technology Madras</td>
<td>5 months</td>
<td>M</td>
<td>Catalytic Fast Pyrolysis of biomass to produce Fuels and chemicals</td>
</tr>
<tr>
<td>Pio Gramazio</td>
<td>University of Bologna</td>
<td>6 months</td>
<td>M</td>
<td>Membrane materials for hydrogen production, Pd based and ceramic membranes</td>
</tr>
<tr>
<td>Wiktor Patura</td>
<td>AGH University</td>
<td>2 weeks</td>
<td>M</td>
<td></td>
</tr>
<tr>
<td>Evangelos Smith</td>
<td>University of Wisconsin Madison</td>
<td>3 months</td>
<td>M</td>
<td></td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>Name</th>
<th>Institution / Country</th>
<th>Year(s)</th>
<th>Type</th>
<th>Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Katarzyna Swirk</td>
<td>NTNU Poland</td>
<td>2020-2023</td>
<td>F</td>
<td>MesoSi-CO(_2). Design of low-cost and carbon-resistant Ni-based mesoporous silicas for chemical CO(_2) utilization through tri-reforming of methane</td>
</tr>
<tr>
<td>Hongfei Ma</td>
<td>NTNU China</td>
<td>2021-2023</td>
<td>M</td>
<td>Chemical transformation of enzymatic hydrolysis lignin (EHL) with catalytic solvolysis to fuel commodities under mild conditions (EHLCATHOL)</td>
</tr>
<tr>
<td>Ainara Moral</td>
<td>NTNU Spain</td>
<td>2021-2023</td>
<td>F</td>
<td>Moving Bed Carbonate Looping</td>
</tr>
<tr>
<td>Felix Herold</td>
<td>NTNU Germany</td>
<td>2021-2023</td>
<td>M</td>
<td>Carbon materials</td>
</tr>
<tr>
<td>Pio Gramazio</td>
<td>NTNU Italy</td>
<td>2023-2025</td>
<td>M</td>
<td>Direct conversion of CO(_2) and hydrogen to fuels</td>
</tr>
<tr>
<td>Izar Capel Berdelle</td>
<td>UiO Spain</td>
<td>2021-2023</td>
<td>M</td>
<td>Catalyst deactivation studies</td>
</tr>
<tr>
<td>Abdulla Bin Afif</td>
<td>UiO India</td>
<td>2023</td>
<td>M</td>
<td>Operando/in-situ Reactor STM and TEM for catalyst development for reactions as ammonia slip and CO(_2) utilization</td>
</tr>
</tbody>
</table>

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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.
# Master's students in Chemical engineering¹ (NTNU) or Chemistry² (UiO) in iCSI

<table>
<thead>
<tr>
<th>Student Name</th>
<th>Institution</th>
<th>Country</th>
<th>Year</th>
<th>Type</th>
<th>Project Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mathilde Ingeborg Nilsen Verne</td>
<td>UiO, iCSI</td>
<td>Norway</td>
<td>2021-2023</td>
<td>F</td>
<td>In-situ XPS of PtRh NPs for NH₃ oxidation</td>
</tr>
<tr>
<td>Daniel Levent Arnes</td>
<td>UiO</td>
<td>Norway</td>
<td>2021-2023</td>
<td>M</td>
<td>Methanol-mediated conversion of CO₂ and H₂ to light hydrocarbons</td>
</tr>
<tr>
<td>Cathinka S. Carlsen</td>
<td>UiO</td>
<td>Norway</td>
<td>2022-2024</td>
<td>F</td>
<td>Platinum group metal transport in ammonia combustion and recovery</td>
</tr>
<tr>
<td>Phillip A. March</td>
<td>UiO</td>
<td>Norway</td>
<td>2022-2024</td>
<td>M</td>
<td>MOF(UIO-66)-Cu(Ni, Au, Pd) nanoparticle hybrid materials for photo- and thermal catalytic conversion of CO₂</td>
</tr>
<tr>
<td>Live Bjernereim Lybekk</td>
<td>UiO</td>
<td>Norway</td>
<td>2022-2024</td>
<td>F</td>
<td>Supported Cu based nanoparticles for thermal- and photo catalysis</td>
</tr>
<tr>
<td>Andrea Kjølén</td>
<td>NTNU</td>
<td>Norway</td>
<td>2022-2023</td>
<td>F</td>
<td>Catalytic pyrolysis of waste plastic to liquids</td>
</tr>
<tr>
<td>Hammad Ali</td>
<td>NTNU</td>
<td>Pakistan</td>
<td>2022-2023</td>
<td>M</td>
<td>Fast Pyrolysis and upgrading of biomass</td>
</tr>
<tr>
<td>Ida Saxrud</td>
<td>NTNU</td>
<td>Norway</td>
<td>2022-2023</td>
<td>F</td>
<td>Catalysts for Syngas Conditioning for Advanced Biofuels</td>
</tr>
<tr>
<td>Tomasz Skrzydło</td>
<td>NTNU, iCSI</td>
<td>Poland</td>
<td>2022-2023</td>
<td>M</td>
<td>Oxidation of methanol to formaldehyde (MTF) over Ag catalyst</td>
</tr>
<tr>
<td>Pål Martin Benum</td>
<td>NTNU, iCSI</td>
<td>Norway</td>
<td>2022-2023</td>
<td>M</td>
<td>Catalytic Oxidation of NO to NO₂ at Industrial Nitric Acid Conditions</td>
</tr>
<tr>
<td>Sahra Louise Guldahl-Ibouder</td>
<td>NTNU</td>
<td>Norway</td>
<td>2022-2023</td>
<td>F</td>
<td>Model catalysts for fundamental insights into the Fischer-Tropsch Synthesis</td>
</tr>
<tr>
<td>Robert Lennard Peters</td>
<td>NTNU</td>
<td>The Netherlands</td>
<td>2022-2023</td>
<td>M</td>
<td>Ketonisation of acetic acid</td>
</tr>
<tr>
<td>Alicia San Martin Rueda</td>
<td>NTNU</td>
<td>Spain</td>
<td>2022-2023</td>
<td>F</td>
<td>Catalysts for advanced biofuels synthesis via the Fischer-Tropsch process</td>
</tr>
<tr>
<td>Nora Nyberget Cornelussen</td>
<td>NTNU</td>
<td>Norway</td>
<td>2023-2024</td>
<td>F</td>
<td>Fast pyrolysis of biomass and catalytic upgrading</td>
</tr>
<tr>
<td>Jørgen Skjæveland</td>
<td>NTNU</td>
<td>Norway</td>
<td>2023-2024</td>
<td>M</td>
<td>Upscaling of biofuel production by hydrodeoxygenation (HDO) of pyrolysis bio-oil</td>
</tr>
<tr>
<td>Sunaina Poonacha Murakatira</td>
<td>NTNU</td>
<td>India</td>
<td>2023-2024</td>
<td>F</td>
<td>Catalytic co-pyrolysis of plastic wastes and biomass to naphtha</td>
</tr>
<tr>
<td>Kai Hoang Dinh</td>
<td>NTNU</td>
<td>Norway</td>
<td>2023-2024</td>
<td>M</td>
<td>Integrated pyrolysis and catalytic upgrading of plastic wastes</td>
</tr>
<tr>
<td>Andrine Jenssen</td>
<td>NTNU</td>
<td>Norway</td>
<td>2023-2023</td>
<td>F</td>
<td>Direct air capture</td>
</tr>
<tr>
<td>Thomas Nhan Nguyen</td>
<td>NTNU</td>
<td>Norway</td>
<td>2023-2024</td>
<td>M</td>
<td>Catalytic purification of pyrolysis oil</td>
</tr>
<tr>
<td>Ingrid Johanne Kausen</td>
<td>NTNU, iCSI</td>
<td>Norway</td>
<td>2023-2024</td>
<td>F</td>
<td>Indium-enhanced iron catalysts for CO₂ Hydrogenation</td>
</tr>
<tr>
<td>Kristin Haukaas Hagen</td>
<td>NTNU, iCSI</td>
<td>Norway</td>
<td>2023-2024</td>
<td>F</td>
<td>Carbon combustion synthesis of a CO₂ to Methanol catalyst</td>
</tr>
<tr>
<td>Sander Ose Velle</td>
<td>NTNU</td>
<td>Norway</td>
<td>2023-2024</td>
<td>M</td>
<td>Pd-alloy catalysts and membranes for hydrogen technology</td>
</tr>
<tr>
<td>Emma Birklund</td>
<td>NTNU</td>
<td>Norway</td>
<td>2023-2024</td>
<td>F</td>
<td>Catalytic Steam Reforming of Hydrocarbon Impurities from Biomass Gasification</td>
</tr>
<tr>
<td>Rebekka Børresen Anda</td>
<td>NTNU</td>
<td>Norway</td>
<td>2023-2024</td>
<td>F</td>
<td>Mesoporous silicas derived from rice husk for chemical CO₂ utilization</td>
</tr>
</tbody>
</table>

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

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### International exchange master’s students associated with iCSI

<table>
<thead>
<tr>
<th>Student Name</th>
<th>Institution</th>
<th>Country</th>
<th>Year</th>
<th>Type</th>
<th>Project Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mei Ju Anne Goemans</td>
<td>Master NTNU</td>
<td>The Netherlands</td>
<td>5 months</td>
<td>F</td>
<td>Cobalt Catalyzed Fischer-Tropsch-Synthesis: Systematic Studies on Carbon Support Effects on Catalyst Activity and Deactivation</td>
</tr>
<tr>
<td>Simon Meilinger</td>
<td>Master NTNU</td>
<td>Germany</td>
<td>2 months</td>
<td>M</td>
<td>Characterisation and Screening of Heteroatom-Doped Carbon Nanofibre Supported Platinum Catalysts for Aqueous Phase Reforming</td>
</tr>
<tr>
<td>Matilde Emanuelli</td>
<td>Bachelor NTNU</td>
<td>Italy</td>
<td>3 months</td>
<td>M</td>
<td>Characterization of silver catalysts surface</td>
</tr>
</tbody>
</table>

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Master’s students from NTNU joined the KinCat (NTNU/SINTEF catalysis group) skiing day in March 2023.
iCSi Invited Plenaries:
Unni Olsbye: Thermodynamic-conversion of CO₂ and H₂ to higher hydrocarbons. 9th North American Catalysis Conference, 2023-04-01 - 2023-04-06
Fjermedt, Torstein; Uglietti, Riccardo; Mcalle, Daniele; Bracconi, Mauro; Phan, Anh; Strollo, Alberto; Iacoviello, Francesco; Svelle, Stian; Maestri, Matteo: Modelling the Methanol to Dimethyl ether reaction – coupling kinetics with transport from CM to a scale. SMN winter seminar, 2023-01-11 - 2023-01-13
Fjermedt, Torstein; Uglietti, Riccardo; Mcalle, Daniele; Bracconi, Mauro; Phan, Anh; Strollo, Alberto; Iacoviello, Francesco; Svelle, Stian; Maestri, Matteo: Modelling the Methanol to Dimethyl ether Reaction – Coupling Kinetics with Transport from CM to a Scale. Guest lecture, IntricateIT 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. LINKS Catalysis Workshop, 2023-05-02 - 2023-05-03

iCSI Publications and conference contributions 2023

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

Journal Publications
Gopakumar, Jithin; Martin Benum, Pål; Svenum, Ingeborg-Helene; Enger, Bjørn Christian; Waller, David; Ranning, 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; Vollum, Per Erik; Ranning, Magnus: Catalytic oxidation of NO to NO₂ for industrial nitric acid production using Ag-promoted MnOx/Al₂O₃ catalysts. Catalysis Science Technology, 2023, 13, 2783-2793
J. Gopakumar, A. Miro i Rovira, B.C. Enger, D. Waller, M. Rønning, Comparison of Ceria-Supported Catalysts for Attaining NO - NO₂ Equilibrium at Industrial Nitric Acid Plant Conditions, 2024 (submitted)
J. Gopakumar, R. Myrstad, R. Barrenes Anda, H. Ølen, B.C. Enger, D. Waller, M. Rønning, Operando Studies of Pt Supported Catalysts at the NOx Catalyst Conversion, 2024 (submitted)
Jithin Gopakumar, NTNU: Ruthenium catalysts to attain NO-NO₂ equilibrium 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 EuropCat 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 WO₃-TiO₂ Monolith Catalysts used for NH₃-SCR of NOx in bio-fuš exhaust gas, 15th EuropCat 2023 Congress, Prague, Czechia, 2023-08-27 - 2023-09-01
Silje F. Håkonsen and Karl Asl 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
Youni van Valen: Effects of Co-feeding reactants in H₂ and CO oxidation over Silver, ICSI Annual seminar, Trondheim, Norway, 2023-06-5 - 2023-06-07
Jasmina H. Cakova, Ole Bjerkedal Håvik, and Ann Kristin Løgmanneve: Main achievements in research and innovation in Industrial Innovation Area 3, ICSI Annual seminar, Trondheim, Norway, 2023-06-5 - 2023-06-07

Posters
Youni van Valen: Oxidation of Methanol to Formaldehyde over Silver Using an Annular Reactor, 15th EuropCat 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; Fenges, Endre; Ma, Hongfei; Sollund, Erling Olov; Margossia, Tigran; Rout, Kumar Ranjan; Chen, De: Promoter doping for tuning the redox behavior of Cu₃Al₄O₉-P₂O₅ based catalysts in ethylene oxychlorination. Insights from kinetic studies, Chemical Engineering Journal 2023, Volume 47, 144593
Zhang, Wei, Ma, Hongfei, Wang, Yalan, Rout, Kumar Ranjan, Margossia, Tigran, Chen, De: Toward Fully Selective Ethylene Oxyclochlorination through Engineering the Cu Oxidation State Spatial Profile, ACS Catalysis 2023, 13, 12, 15107-15114
Hongfei Ma, Xiuhi Zheng, Hao Zhang, Guoyan Mo, Wei Zhang, Zheng Jiang, De Chen: Atomic Cu-N-P-C Active Complex with Integrated Oxidation and Chlorination for Improved Ethylene Oxyclochlorination, Advanced Science, 2023, Volume 10(8), 2205635
Zhang, Wei, Ma, Hongfei, Wang, Yalan, Regli, Samuel K.; Ranning, Magnus; Rout, Kumar Ranjan; Margossia, Tigran; Chen, De: In situ monitoring of dynamic behavior of La-doped Cu₃Al₄O₉-P₂O₅ catalyst in ethylene oxyclochlorination. Journal of Catalysis 2023; Volume 417, 314-322

Oral Presentations
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