Photocatalysis of methane using non-noble metal oxides

Trial lecture

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11.08.2023
iCSI Partners

Norwegian Centre for Research-based Innovation

NTNU  SINTEF  UiO: University of Oslo

TOPSOE  INEOS Inovyn

YARA

KA-Rasmussen  Dyna

Funded by The Research Council of Norway

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 Banning 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.

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

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

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

The representation on the iCSI Board has changed for one of the industry partners in 2023, with Ann Kristin Laggansveen 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!

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

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

Cover photo: PhD candidate Karoline Kvande at the defense of her PhD thesis August 11, 2023. Photo: Private
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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 Topsøe A/S – also conduct their own significant R&D. The collaboration enables the optimized use of complementary competence and a shared, highly advanced, experimental infrastructure that is being utilized, expanded and developed within iCSI. The research is organized into 6 Industrial Innovation Areas (IIA1-6), each with 1-6 work packages. Cutting-edge research topics addressing the key challenges are identified for each of the iCSI industrial innovation areas (IIA1-5) and defined as Work Packages. IIA6 is focusing on the development of methodology in line with the international forefront, and these methods are gradually being integrated into the activities of IIA1-5. Each IIA has 2-3 research partners and 1-2 industrial partners, while IIA6 is generic and involves all the partners.

Industrial Partners

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

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

K.A. Rasmussen 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 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 well-known 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 Topsoe 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 iCSI’s internationalization and recognition.

Management and Administration

The Centre is hosted by the Department of Chemical Engineering at NTNU. The administration team consists of a Centre Director, a Coordinator/Vice Director (50% position) and an Economy Advisor (20% position).
As the last in the series of portraits of professors in the iCSI family, Centre Director Hilde Johnsen Venvik will this year tell a little about herself and her motivation for carrying out catalysis research.

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

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

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

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

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

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

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

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

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

There are two messages she repeats to all students:
- You must carefully consider how catalyst activity is defined and measured
- You have to think through what a measurement actually means (what is perturbation and response and what can be interpreted - and NOT interpreted - out of it).

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

iCSI is now shutting down as a centre after eight years. What has been the most fun while leading it? “It has been the interaction with and appreciation from the inspirational competent industrial partners, the collaborative spirit existing between the research groups, and seeing the PhD candidates develop and complete their research.

At iCSI, we have achieved almost everything I hoped for when we started in 2015 - in education, publishing and research. The resulting innovations are more difficult to document or predict, but we have contributed a lot of new knowledge that the industry will make use of in various ways, in addition to a small number of patenting initiatives. We could possibly have been better at popularising our results, but we have had individuals who have demonstrated both the will and good ability to do this.”

Hilde also insists on adding that SFI is a unique instrument for innovation-driven research in a national and international context. She believes that history will show that it has been more important than what we see and are able to document today.

“Artificial intelligence (AI) is predicted to change our world in dramatic ways. What possibilities does Hilde envision with this tool - for better or for worse?” “The possibility of insight (science) and profit (business) is enormous if you are able to use it to connect data, physical properties and theoretical models. This involves quite extreme system-
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.
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 (microlorimetry). 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 microlorimetry 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); Izá Capel Berdeill (iCSI Postdoc); Pablo Beato (senior scientist at Haldor Topsøe A/S); Bjørn Gading Solemsli (iCSI PhD candidate); Izar Capel Berdiell (iCSI Postdoc); Pablo Beato (senior scientist at Haldor Topsøe A/S); Bjørn Gading Solemsli (iCSI Centre Director); Karoline Kvande (iCSI PhD candidate); Izar Capel Berdeill (iCSI Postdoc); Pablo Beato (senior scientist at Haldor Topsøe A/S); Bjørn Gading Solemsli (iCSI Centre Director); Karoline Kvande (iCSI PhD candidate); Izar Capel Berdeill (iCSI Postdoc); Pablo Beato (senior scientist at Haldor Topsøe A/S); Bjørn Gading Solemsli (iCSI Centre Director).**
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 production of nitric acid, which 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 oxidation of NO in the gaseous phase (NO2) and the subsequent reaction of NO2 with water produces nitric acid. O2, He, and H2 are present in the reactor gas. Further, NO2 is 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.

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

The results reveal the mechanism behind NO oxidation at industrial nitric acid production conditions over γ-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 1  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

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

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
iCSI Concluding Seminar

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

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

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

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

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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<td>Lunch@Realfagskantina</td>
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<tr>
<td>13:00-13:15</td>
<td>Pablo Beato, Topse, Chair of the iCSI Board</td>
<td>Welcome to seminar</td>
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<td>13:15-13:40</td>
<td>IAI: Anja O. Sjøstad, UIO and David Waller, Yara</td>
<td>Main achievements in research and innovation</td>
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<td>13:40-14:00</td>
<td>IAI: Sjile F. Håkonsen, SINTEF and Karl Isak Skau, Yara</td>
<td>Main achievements in research and innovation</td>
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<td>14:00-14:25</td>
<td>IAI: Jasmina H. Cavka, SINTEF, Ole Bjerkedal Håvik, Dynes and Ann Kristin Lagmannsveen, K. A. Rasmussen</td>
<td>Main achievements in research and innovation</td>
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<td>14:25-14:45</td>
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<td>14:45-15:10</td>
<td>IAI: De Chen, NTNU</td>
<td></td>
</tr>
<tr>
<td>15:10-15:35</td>
<td>IAI: Stian Svelle, Univ. of Oslo</td>
<td></td>
</tr>
<tr>
<td>15:35-16:00</td>
<td>IAI: Magnus Ramming, NTNU</td>
<td></td>
</tr>
<tr>
<td>16:22</td>
<td>Casual dining @Hilde’s garden in Sleipnes vei 5</td>
<td></td>
</tr>
</tbody>
</table>

Day 2  Tuesday June 6 iCSI seminar, guest from CATHEX are welcome to join, 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>Edd Blekkan, NTNU</td>
<td>Welcome</td>
</tr>
<tr>
<td>09:10-09:30</td>
<td>Jinlin 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>Yousi van Valen, NTNUUnw</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>Coffee break</td>
<td></td>
</tr>
<tr>
<td>10:50-11:10</td>
<td>Bjørn Gading Sølemsi, Univ. of Oslo</td>
<td>Methylation versus oligomerization of light Aikenes and Benzene through stepwise reaction with Methane in Cu-Exchanged Zeolites.</td>
</tr>
<tr>
<td>11:10-11:25</td>
<td>Dimitrius Pappas, CoorsTek</td>
<td>Experiences after ICSI</td>
</tr>
<tr>
<td>11:25-11:40</td>
<td>Aase Marie Hunde, 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 Iglesas, 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, Topse</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>Celebration dinner@NINA-kantina</td>
<td></td>
</tr>
</tbody>
</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>09:10-09:30</td>
<td>Ja Yang, Shanghai Jiao Tong Univ.</td>
<td>Iron based Fischer Tropsch synthesis</td>
</tr>
<tr>
<td>09:50-10:30</td>
<td>Manos Mavrikakis, 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 Alkane 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. Sjøstad, 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 Claeyts, 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 Huy, 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 Proodinger, 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 Tingstadv, NTNU</td>
<td>Welcome</td>
</tr>
<tr>
<td>09:10-09:40</td>
<td>Prof. Magnus Ramming, 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 Ilyshe, NTNU</td>
<td>Hydrotricalte-Derived Nickel-Cobalt Catalysts for Steam Reforming of Bio-Syngas Hydrocarbon Impurities</td>
</tr>
<tr>
<td>09:50-10:00</td>
<td>Oscar Luis Ianez 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]) 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 coking 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>Ainara Moral Larrasannna, 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 for C-O Formation and 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 Replace ment via Gasification-Assisted Heteratom 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 hydro gen sensors</td>
</tr>
<tr>
<td>12:10-12:20</td>
<td>Monica Pazos Urrea, NTNU</td>
<td>Utilizing carbon nanofiber-supported catalysts for hydrogen prod uction via aqueous phase reforming of ethylene glycol</td>
</tr>
<tr>
<td>12:20-12:30</td>
<td>Albert Miro i Rovira, NTNU</td>
<td>Hydrodeoxygenation of bio- oil</td>
</tr>
<tr>
<td>12:30-13:30</td>
<td>Lunch</td>
<td></td>
</tr>
<tr>
<td>13:30</td>
<td>Social activities (optional )</td>
<td></td>
</tr>
</tbody>
</table>
Scientific Activities
Scientific Activities

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

### IIA1

21st Century Ammonia Oxidation and Nitric Acid technology development

- **WP1.1**
  - NTNU
  - SINTEF
  - YARA
  - University of Oslo

- **WP1.2**
  - University of Oslo

- **WP1.3**
  - NTNU
  - SINTEF
  - YARA
  - University of Oslo

### IIA2

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

- **WP2.1**
  - SINTEF
  - YARA

### IIA3

Frontier formalin technology development

- **WP3.1**
  - NTNU
  - SINTEF

- **WP3.2**
  - SINTEF

- **WP3.3**
  - SINTEF

### IIA4

PVC Value Chain: World class energy production of Chlorine and Vinyl Chloride Monomer (VCM)

- **WP4.1**
  - NTNU
  - SINTEF

- **WP4.2**
  - SINTEF

- **WP4.3**
  - INEOS

- **WP4.4**
  - YARA

- **WP4.5**
  - YARA

### IIA5

The next step in direct activation of lower alkanes

- **WP5.1**
  - TOPSOE
  - SINTEF
  - University of Oslo

- **WP5.2**
  - SINTEF

- **WP5.3**
  - SINTEF

### IIA6

Generic projects for additional industrial synergies

- **WP6.1**
  - NTNU
  - SINTEF

- **WP6.2**
  - SINTEF

- **WP6.3**
  - SINTEF

- **WP6.4**
  - SINTEF

- **WP6.5**
  - SINTEF

- **WP6.6**
  - SINTEF

- **WP6.7**
  - NTNU

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

The IIA1 team 2023

<table>
<thead>
<tr>
<th>Name</th>
<th>Institution</th>
<th>Role</th>
</tr>
</thead>
<tbody>
<tr>
<td>Anja Olafsen Sjåstad</td>
<td>UiO</td>
<td>IIA leader, PhD supervisor and WP responsible (WP1.1), advisor (WP1.2)</td>
</tr>
<tr>
<td>Helmer Fjellvåg</td>
<td>UiO</td>
<td>Advisor (WP1.1-1.2)</td>
</tr>
<tr>
<td>Julie Hessevik</td>
<td>UiO</td>
<td>PhD candidate (WP1.1)</td>
</tr>
<tr>
<td>Martin Jensen</td>
<td>UiO</td>
<td>Researcher (WP1.1)</td>
</tr>
<tr>
<td>Henrik Sætøby</td>
<td>UiO</td>
<td>Researcher (WP1.1)</td>
</tr>
<tr>
<td>Cathinka S. Carlsen</td>
<td>UiO</td>
<td>Master's student (WP1.1)</td>
</tr>
<tr>
<td>David Waller</td>
<td>YARA</td>
<td>Industry senior researcher (WP1.1-1.2-1.3), PhD supervisor (WP1.1)</td>
</tr>
<tr>
<td>Danielle Farmer</td>
<td>YARA</td>
<td>Industry researcher (WP1.1)</td>
</tr>
<tr>
<td>Oskar Iveland</td>
<td>YARA</td>
<td>Industry researcher (WP1.1)</td>
</tr>
<tr>
<td>Marianne S. Granvold</td>
<td>YARA</td>
<td>Industry researcher (WP1.1)</td>
</tr>
<tr>
<td>Torgeri Lunde</td>
<td>YARA</td>
<td>Industry senior</td>
</tr>
<tr>
<td>Ann Kristin Lagmannsveen</td>
<td>KA Rasmussen</td>
<td>Industry Researcher (WP1.1-1.2)</td>
</tr>
<tr>
<td>Federica Mudu</td>
<td>KA Rasmussen</td>
<td>Industry Researcher (WP1.1-1.2)</td>
</tr>
<tr>
<td>Silje Fosse Håkonsen</td>
<td>SINTEF</td>
<td>Researcher WP responsible (WP1.2)</td>
</tr>
<tr>
<td>Bærge Holme</td>
<td>SINTEF</td>
<td>Researcher (WP1.2)</td>
</tr>
<tr>
<td>Martin F. Sunding</td>
<td>SINTEF</td>
<td>Researcher (WP1.2)</td>
</tr>
<tr>
<td>Kari Anne Andreassen</td>
<td>SINTEF</td>
<td>Senior Engineer (WP1.2)</td>
</tr>
<tr>
<td>Joanna Pičhala</td>
<td>SINTEF</td>
<td>Research engineer (WP1.2)</td>
</tr>
<tr>
<td>Magnus Ramming</td>
<td>NTNU</td>
<td>PhD supervisor, WP responsible (WP1.3)</td>
</tr>
<tr>
<td>Jithin Gopalakumar</td>
<td>NTNU</td>
<td>PhD candidate (WP1.3)</td>
</tr>
<tr>
<td>Fål Martin Benum</td>
<td>NTNU</td>
<td>Master's student (WP1.3)</td>
</tr>
<tr>
<td>Rune Lødeng</td>
<td>SINTEF</td>
<td>PhD supervisor, senior researcher (WP1.3)</td>
</tr>
<tr>
<td>Bjørn Christian Enger</td>
<td>SINTEF</td>
<td>Senior researcher (WP1.3)</td>
</tr>
</tbody>
</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 Pt 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.
IIA2: Abatement of Nitrogen-containing Pollutants – State-of-the-art Catalyst Technology

The IIA2 team 2023

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

Motivation

When ammonia is combusted in a nitric acid plant in the Oswald process to produce NOx, N2O is an unwanted byproduct. 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.

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.

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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.
IIA3: Frontier Formalin Technology Development

The IIA3 team 2023

Jasmina Hafizovic Cavka SINTEF IIA leader

Hilde Venvik NTNU PhD supervisor, WP responsible (WP3.1), advisor (WP3.3)

Jia Yang NTNU PhD co-supervisor (WP3.1), advisor (WP3.3)

Youri van Valen NTNU PhD candidate (WP3.1)

Matilde Emanuelli NTNU Exchange bachelor’s student (WP3.1)

Tina Bergh NTNU Postdoctoral fellow (WP3.1/WP6.7)

Tomasz Skrzydlo NTNU Master’s student (WP3.1)

Ann Kristin Lagnannsveen KA Rasmussen Industry researcher (WP3.1)

Federica Mudu KA Rasmussen Industry researcher (WP3.1)

Ole H. Bjørkedal DYNEA Industry researcher (WP3.1-3.2-3.3), WP responsible (WP3.2)

Lars Axelsen DYNEA Industry senior (WP3.1-3.2)

Rune Ladeng SINTEF PhD co-supervisor (WP3.1), senior researcher (WP3.2-3.3)

Roman Tschentscher SINTEF Senior researcher (WP3.2-3.3)

Kari Anne Andreassen SINTEF Senior engineer (WP3.3)

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

In IIA3, we study annular and particulate silver catalysts used for the partial oxidation of methanol (CH\textsubscript{3}OH) and its relevant sub-reactions, for example oxidation of CO and H\textsubscript{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. Image processing is done to enhance the pore edges, as exemplified in (h). Finally, we plot the (sub-)surface pores in 3D, as shown in (j). Several large, faceted pores can be seen extending beyond 25 μm into the silver. We believe that this is due to the dissolution of oxygen and hydrogen in the silver crystal lattice and their subsequent recombination, together with a high mobility of silver atoms at high temperature. We also compliment the slice-and-view with electron backscatter diffraction (EBSD) data collected at different stages during the milling, to extract the local crystallographic orientation across the polished surfaces. Furthermore, we use the FIB to prepare cross-sectional lamellae for (scanning) transmission electron microscopy (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.
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, CsCl, CrCl3, NdCl3, ErCl3, FeCl3, YCl3, and SnCl3) on the CuCl2/y-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/y-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/y-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 KMgLa-CuCl2/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/y-Al2O3-based catalysts at 220−260°C and low pressure (1−5 bar), characteristic of a highly exothermic reaction. This EDC is subsequently cracked to VCM, endothermically at 500−550 °C and higher pressure (15−20 bar). The VCM selectivity exceeds 90%, but the conversion remains at around 50%. This is an energy-intensive process.

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 C* on the surface. HCl is dissociated with O* and the formed C* can directly react with C2H4* forming C2H3Cl* (EDC*). The adsorbed EDC* prefers to undergo the dehydrochlorination reaction to VCM* and HCl*, which can continue to react in the next cycle with O*. This work highlights how rational design of 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 Prodinge 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 Zingler Stummann Haldor Topsøe A/S Industry researcher (WPS.1-5.2-5.3)
Bjørnar Arstad SINTEF Senior researcher (WPS.5.3)

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.

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.

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

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

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

PhD candidate Bjørn Gading Solemsli presenting his results at the ICSI/CATHEX seminar in June 2023.
IIA 6: Generic Projects for Additional Industrial Synergies

The IIA6 team 2023

<table>
<thead>
<tr>
<th>Name</th>
<th>Institution</th>
<th>Position/Role</th>
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<tbody>
<tr>
<td>Magnus Rønning</td>
<td>NTNU</td>
<td>IIA leader, PhD supervisor and WP responsible (WP6.1)</td>
</tr>
<tr>
<td>Hilde Johnsen Venvik</td>
<td>NTNU</td>
<td>PhD co-supervisor (WP6.1) and postdoc supervisor (WP6.7)</td>
</tr>
<tr>
<td>Samuel K. Regli</td>
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<td>PhD candidate (WP6.1)</td>
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<tr>
<td>Anja Olafsen Sjåstad</td>
<td>UiO</td>
<td>WP responsible (WP6.2)</td>
</tr>
<tr>
<td>Martin Jensen</td>
<td>UiO</td>
<td>PhD candidate, associated (WP6.2)</td>
</tr>
<tr>
<td>Mathilde Ingeborg N. Verne</td>
<td>UiO</td>
<td>Master’s student (WP6.2)</td>
</tr>
<tr>
<td>Evgeniy Redekop</td>
<td>UiO</td>
<td>Researcher (WP6.2)</td>
</tr>
<tr>
<td>Bjørn Christian Elger</td>
<td>SINTEF</td>
<td>WP responsible and senior researcher (WP6.4)</td>
</tr>
<tr>
<td>Ingeborg-Helene Svenum</td>
<td>SINTEF</td>
<td>Researcher (WP6.4)</td>
</tr>
<tr>
<td>Edd A. Blekkan</td>
<td>NTNU</td>
<td>WP responsible (WP6.5 ) and PhD supervisor (WP6.5) and co-supervisor (WP6.6)</td>
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<tr>
<td>Jia Yang</td>
<td>NTNU</td>
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<tr>
<td>De Chen</td>
<td>NTNU</td>
<td>PhD co-supervisor (WP6.5 and 6.6)</td>
</tr>
<tr>
<td>Moses Mawanga</td>
<td>NTNU</td>
<td>PhD candidate (WP6.5)</td>
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<tr>
<td>Bjorn Frederik Baumgarten</td>
<td>NTNU</td>
<td>PhD candidate (WP6.6)</td>
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<tr>
<td>Ingrid Johanne Paulsen</td>
<td>NTNU</td>
<td>Master’s student (WP6.6)</td>
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<td>Kristin Haukaas Hagen</td>
<td>NTNU</td>
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<tr>
<td>Rune Laedeng</td>
<td>SINTEF</td>
<td>Senior researcher (WP6.6)</td>
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<tr>
<td>Tina Bergh</td>
<td>NTNU</td>
<td>Postdoctoral fellow (WP6.7)</td>
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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 know-how about how process temperature, gas atmosphere and nanoparticle size dictate the Pt-Rh element distribution are prerequisites. With this motivation, we mapped the element distribution in Pt-Rh nanoparticles with a 50-50 at.% Pt-Rh versus temperature and nanoparticle size using in-situ TEM (HAADF-STEM) at vacuum conditions.

The in-situ TEM experiments were carried out between room temperature and 650 °C to elucidate the tendency of elemental mixing/segregation with respect to nanoparticle size and temperature for particles ≤ 24 nm. The study fully relies on well-defined 50-50 at.% Pt-Rh solid solution and Rh(core)-Pt(shell) nanoparticles synthesised by means of colloidal routes in our own laboratory (Jensen, M., et al. Innovative approach to controlled Pt–Rh bimetallic nanoparticle 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 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

\[
\Delta m = K_0 \left( \frac{1}{f_1^2} - \frac{1}{f_2^2} \right)
\]

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 near 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.
Hosted 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/student exchanges 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.

### Internationalization

#### Overview of international collaborations:

**Universities and Institutes**
- Aalto University, Finland
- Agile 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 (Huazhon), China
- CNRS, 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
- Institut National de l’Carbón, INCAR-CSIC, Spain
- Karlsruhe Institute of Technology – KIT, Germany
- KAUST, Saudi Arabia
- Kemijski Institutu – NIC, Slovenia
- Luleå University of Technology, Sweden
- Lund University, Sweden
- Manchester Metropolitan University, United Kingdom
- MAX IV Laboratory, Lund, Sweden
- Mas Planck Institute for Energy Conversion, Germany
- Norner Research AS (SCG Chemicals), Norway
- Paul Sherrer Institut, Switzerland
- Polytechnic University of Catalunya, Spain
- Politecnico di Milano, Italy
- Research Institutes of Sweden (RISE), Sweden
- School of Chemistry and Chemical Engineering, Shanghai Jiao Tong University, China
- Shansi 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 De 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
- Arkena France SA, France
- B.T.G. BV, Netherlands
- Borealis Polyolefine, Austria
- BTG-BTL, Belgium
- C2P2, Lyon (CNRS), France
- Eiken Silicon Materials, Norway/France
- Equinor, Norway (med?)
- Firmenich, Switzerland
- ICI Caldaie, Italy
- ILS, Integrated Lab Solutions, Germany
- Johnson Matthey, United Kingdom
- Linde, Germany
- Neste, Finland
- NextChem SPA, Italy
- OMV, Austria
- Process design center B.V. (PDC), Netherlands
- Rando, Czech Republic
- Repsol SA, Spain
- Siemens Energy, Sweden
- Steeper, Denmark
- Tata Steel UK Limited, UK
- Toppso AS, Denmark
- TotalEnergies, France
- Turkiye Petrol Rafinerileri Anonim Sirketi (Tüpraş), Turkey
- UOP LLC, USA
- VTT, Finland

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**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.

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In 2023, Hilde Venvik finalised the three-year period as Lise Meitner-professor at the Department of Chemical Engineering at Lund University.
European research - Horizon 2020 and Horizon Europe project


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


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.


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


International collaborations supported by RCN and sources other than EU


CATHEX - Advances in heterogeneous catalysis through integrated theoretical and experimental efforts. h2022-3-TWIN-TRANSITION-01-1, iCSI-partners involved: SINTEF, 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. Durations: 2021-2023.


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


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 Rupprechter, TU Wien were shown the experimental rigs in the NTNU laboratories.

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Accounts 2023

All cost and budget numbers appear in 1000 Norwegian Kroner, NOK, as of March 2024. NOK 100 are equivalent to €8.7.

Table 1 summaries 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>
</tr>
</thead>
<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><strong>Totals</strong></td>
<td><strong>24 135</strong></td>
<td><strong>196 760</strong></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 2023</th>
<th>Financing</th>
</tr>
</thead>
<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>
</tr>
<tr>
<td>SINTEF</td>
<td>4 902</td>
<td>43 611</td>
<td>7 942</td>
<td></td>
</tr>
<tr>
<td>Research Council of Norway</td>
<td>2 885</td>
<td>5 396</td>
<td>26 502</td>
<td>50 502</td>
</tr>
<tr>
<td><strong>Totals</strong></td>
<td><strong>24 135</strong></td>
<td><strong>24 135</strong></td>
<td><strong>196 760</strong></td>
<td><strong>196 760</strong></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 abatements 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 Catalysis</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><strong>Totals</strong></td>
<td><strong>24 135</strong></td>
<td><strong>196 760</strong></td>
</tr>
</tbody>
</table>

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>

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 | NTNU | Switzerland | 2016-2019 | M | IIAS |
| Moses Mawanga | NTNU | Uganda | 2018-2021 | M | IIAS |
| Karoline Kvanne | UiO | Norway | 2019-2022 | F | IIAS |
| Julie Hessevik | UiO | Norway | 2019-2023 | F | IIA1 |
| Wei Zhang | NTNU | China | 2020-2023 | F | IIAS |
| Jithin Gopakumar | NTNU | India | 2020-2024 | M | IIA1 |
| Youri van Valen | NTNU | Netherlands | 2020-2024 | M | IIA3 |
| Bjørn Gading Solemsli | UiO | Norway | 2021-2024 | M | IIA5 |
| Bjørn Frederik Baumgarten | NTNU | Germany | 2021-2024 | M | IIA6 |

1) Granted by ICSI 8 months in 2023

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 Kvanne’s defense took place 08.08.2023.
4) Wei Zhang’s defense took place 17.11.2023.
5) Julie Hessevik, 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

Postdoc Sebastian Prodinger giving a lecture at ICSI’s finalising seminar in June.

Education

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<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>

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| Moses Mawanga | NTNU | Uganda | 2018-2021 | M | IIAS |
| Karoline Kvanne | UiO | Norway | 2019-2022 | F | IIAS |
| Julie Hessevik | UiO | Norway | 2019-2023 | F | IIA1 |
| Wei Zhang | NTNU | China | 2020-2023 | F | IIAS |
| Jithin Gopakumar | NTNU | India | 2020-2024 | M | IIA1 |
| Youri van Valen | NTNU | Netherlands | 2020-2024 | M | IIA3 |
| Bjørn Gading Solemsli | UiO | Norway | 2021-2024 | M | IIA5 |
| Bjørn Frederik Baumgarten | NTNU | Germany | 2021-2024 | M | IIA6 |

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Postdoc Sebastian Prodinger giving a lecture at ICSI’s finalising seminar in June.
**PhD candidates working on projects in iCSI with financial support from other sources**

<table>
<thead>
<tr>
<th>Candidate</th>
<th>Institution</th>
<th>Country</th>
<th>Start-Year</th>
<th>End-Year</th>
<th>Type</th>
<th>Project Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Ole H. Bjerkedal</td>
<td>NTNU</td>
<td>Norway</td>
<td>2016-2020</td>
<td>M</td>
<td></td>
<td>Selective catalytic reduction (SCR) of NOₓ emissions in maritime transport.</td>
</tr>
<tr>
<td>Martina Cazzolaro</td>
<td>NTNU</td>
<td>Italy</td>
<td>2017-2020</td>
<td>F</td>
<td></td>
<td>Cu/CNF for selective hydrogenation of hydroxyacetone to 1,2-propanediol.</td>
</tr>
<tr>
<td>Jibin Antony</td>
<td>NTNU</td>
<td>India</td>
<td>2018-2022</td>
<td>M</td>
<td></td>
<td>Nanostructured hybrid catalysts for photocatalytic applications.</td>
</tr>
<tr>
<td>Mario Ernesto Casalegno</td>
<td>NTNU</td>
<td>Mexico</td>
<td>2018-2022</td>
<td>M</td>
<td></td>
<td>Catalyst for onboard hydrogen generation from bioethanol.</td>
</tr>
<tr>
<td>Dumitrita Spinu</td>
<td>NTNU</td>
<td>Romania</td>
<td>2019-2022</td>
<td>F</td>
<td></td>
<td>Low temperature CO₂ capture.</td>
</tr>
<tr>
<td>Monica Pazos Urrea 1)</td>
<td>NTNU</td>
<td>Columbia</td>
<td>2020-2023</td>
<td>F</td>
<td></td>
<td>Kinetic studies of aqueous phase reforming including deactivation studies.</td>
</tr>
<tr>
<td>Petter Tingelstad</td>
<td>NTNU</td>
<td>Norway</td>
<td>2020-2023</td>
<td>M</td>
<td></td>
<td>Catalytic upgrading of bio-oil to aviation fuels.</td>
</tr>
<tr>
<td>Oscar Ivanez Encinas</td>
<td>NTNU</td>
<td>Spain</td>
<td>2020-2023</td>
<td>M</td>
<td></td>
<td>Biofuels production from Biomass.</td>
</tr>
<tr>
<td>Kishore Rajendran</td>
<td>NTNU</td>
<td>India</td>
<td>2020-2023</td>
<td>M</td>
<td></td>
<td>Development of efficient catalyst for conversion of biomass to aviation fuel.</td>
</tr>
<tr>
<td>Albert Miró i Revira</td>
<td>NTNU</td>
<td>Spain</td>
<td>2021-2024</td>
<td>M</td>
<td></td>
<td>Catalytic upgrading of bio-oil to aviation fuels.</td>
</tr>
<tr>
<td>Zhihui Li</td>
<td>NTNU</td>
<td>China</td>
<td>2021-2024</td>
<td>F</td>
<td></td>
<td>Conversion of biomass and plastic wastes.</td>
</tr>
<tr>
<td>Sahra Louise Guldahl-Ibouder</td>
<td>NTNU</td>
<td>Norway</td>
<td>2023-2026</td>
<td>F</td>
<td></td>
<td>Development of novel materials for low-temperature ammonia cracking.</td>
</tr>
<tr>
<td>Alicia San Martin Rueda</td>
<td>NTNU</td>
<td>Spain</td>
<td>2023-2026</td>
<td>F</td>
<td></td>
<td>In-situ characterisation of perovskites using advanced techniques.</td>
</tr>
<tr>
<td>Hammad Ali</td>
<td>NTNU</td>
<td>Pakistan</td>
<td>2023-2026</td>
<td>M</td>
<td></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</td>
<td>The Nether-</td>
<td>lands</td>
<td>2023-2026</td>
<td>F</td>
<td>Direct conversion of CO₂ and hydrogen to fuels.</td>
</tr>
<tr>
<td>Vladyslav Shostak</td>
<td>UiO</td>
<td>Ukraine</td>
<td>2020-2023</td>
<td>M</td>
<td></td>
<td>Development of comprehensive diffusion/adsorption models for TAP kinetic experiments.</td>
</tr>
<tr>
<td>Dag Sannes</td>
<td>UiO</td>
<td>Norway</td>
<td>2020-2023</td>
<td>M</td>
<td></td>
<td>Rational design of MOF catalysts for CO₂ conversion.</td>
</tr>
<tr>
<td>Claudia Fabris</td>
<td>UiO</td>
<td>Italy</td>
<td>2022-2025</td>
<td>F</td>
<td></td>
<td>Operando studies of zeolite catalysts.</td>
</tr>
<tr>
<td>Agnieszka Seremak</td>
<td>UiO</td>
<td>Poland</td>
<td>2022-2025</td>
<td>F</td>
<td></td>
<td>Diffusion, reaction, and entropy in zeolites.</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>Candidate</th>
<th>Institution</th>
<th>Country</th>
<th>Start-Year</th>
<th>End-Year</th>
<th>Type</th>
<th>Project Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Nikhil Kumar</td>
<td>Indian Institute of Technology Madras</td>
<td>India</td>
<td>2020-2023</td>
<td>M</td>
<td></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>Italy</td>
<td>2020-2023</td>
<td>M</td>
<td></td>
<td>Membrane materials for hydrogen production, Pt based and ceramic membranes.</td>
</tr>
<tr>
<td>Wiktor Pacura</td>
<td>AGH University</td>
<td>Poland</td>
<td>2020-2023</td>
<td>M</td>
<td></td>
<td>Low temperature CO₂ capture.</td>
</tr>
<tr>
<td>Evangelos Smith</td>
<td>University of Wisconsin Madison</td>
<td>USA</td>
<td>2020-2023</td>
<td>M</td>
<td></td>
<td>Hydrogen membrane separation technology.</td>
</tr>
</tbody>
</table>

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

<table>
<thead>
<tr>
<th>Candidate</th>
<th>Institution</th>
<th>Country</th>
<th>Start-Year</th>
<th>End-Year</th>
<th>Type</th>
<th>Project Description</th>
</tr>
</thead>
<tbody>
<tr>
<td>Katarzyna Swirk</td>
<td>NTNU</td>
<td>Poland</td>
<td>2020-2023</td>
<td>F</td>
<td></td>
<td>Mesocel-CO₂: Design of low-cost and carbon-resistant Ni-based mesoporous silicas for chemical CO₂ utilization through tri-reforming of methane.</td>
</tr>
<tr>
<td>Hongfei Ma</td>
<td>NTNU</td>
<td>China</td>
<td>2021-2023</td>
<td>M</td>
<td></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</td>
<td>Spain</td>
<td>2021-2023</td>
<td>M</td>
<td></td>
<td>Moving Bed Carbone Looping.</td>
</tr>
<tr>
<td>Felix Herold</td>
<td>NTNU</td>
<td>Germany</td>
<td>2021-2023</td>
<td>M</td>
<td></td>
<td>Carbon materials.</td>
</tr>
<tr>
<td>Pio Gramazio</td>
<td>NTNU</td>
<td>Italy</td>
<td>2023-2025</td>
<td>M</td>
<td></td>
<td>Direct conversion of CO₂ and hydrogen to fuels.</td>
</tr>
<tr>
<td>Izar Capel Berdiell</td>
<td>UiO</td>
<td>Spain</td>
<td>2021-2023</td>
<td>M</td>
<td></td>
<td>Catalyst deactivation studies.</td>
</tr>
<tr>
<td>Abdulla Bin Afif</td>
<td>UiO</td>
<td>India</td>
<td>2023</td>
<td>M</td>
<td></td>
<td>Operando/in-situ Reactor STM and TEM for catalyst development for reactions as ammonia slip and CO₂ utilization.</td>
</tr>
</tbody>
</table>
### Master's students in Chemical engineering¹ (NTNU) or Chemistry² (UiO) in iCSI

<table>
<thead>
<tr>
<th>Name</th>
<th>Institution</th>
<th>Country</th>
<th>Year</th>
<th>Gender</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 Kjæri</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 Corneliusen</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 Skjøveland</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 Murukatira</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>2023-2024</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>
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<tr>
<td>Ingrid Johanne Kalsen</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>Rebecca Bærresen 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>Name</th>
<th>Institution</th>
<th>Country</th>
<th>Year</th>
<th>Gender</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>
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<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>Characterisation 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.
Communication and Dissemination 2023

iCSI Invited Plenaries:
Unni Olsbye: Thermo-catalytic conversion of CO₂ and H₂ to higher hydrocarbons. 9th UK Catalysis Conference, 2023-01-04 - 2023-01-06

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

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

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

Magnus Rønning: Operando characterisation of catalysts in demanding sample environments. 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 Benven, Pål; Svennum, Ingeborg-Helene; Enger, Bjørn Christian; Waller, David; Rønning, Magnus: Redox transformations of Ru catalyst during NO oxidation at industrial nitric acid production conditions. Chemical Engineering Journal 2023, Volume 475, 146406
Gopakumar, Jithin; Vold, Sunniva; Enger, Bjørn Christian; Waller, David; Vullum, Per Erik; Rønning, Magnus: Catalytic oxidation of NO to NO₂ for industrial nitric acid production using Ag-promoted MnOₓ/γ-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. Øien, B.C. Enger, D. Waller, M. Rønning: Catalysis of Nitric Oxide Reduction by Catalytic Oxidation of Nitric Oxide, 2024 (submitted)

Oral Presentations
Jithin Gopakumar, NTNU: Ruthenium catalysts to attain NO-NO₂ equilibria at industrial nitric acid conditions, iCSI Annual seminar, Trondheim, Norway, 2023-06-5 - 2023-06-07
Anja O. Sjåstad: Main achievements in research and innovation in Industrial Innovation Area 1, iCSI Annual seminar, Trondheim, Norway, 2023-06-5 - 2023-06-07
Anja O. Sjåstad: On the ammonia oxidation reaction, iCSI and CATHEX seminar, Trondheim 2023-06-05-2023-06-08

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

IIA2: Abatement of nitrogen-containing pollutants. State-of-the-art catalyst technology
Oral Presentations
Sille F. Håkonsen: Phosphorous contamination of a VWO₂-TiO₂ Monolith Catalysts used for NHSCR of NOx in biofuel exhaust combustion, 15th Europacat Congress, Prague, Czechia, 2023-08-27 - 2023-09-01
Sille F. Håkonsen and Karl Isaak 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
Yuori 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. Cava, Ole Bjørkedal Håvåg, and Ann Kristin Lagganmannew: Main achievements in research and innovation in Industrial Innovation Area 3, ICSI Annual seminar, Trondheim, Norway, 2023-06-5 - 2023-06-07

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

IIA4: PVC Value Chain: World Class Energy and Raw Material Efficiency for the Production of Chlorine and Vinyl Chloride Monomer (VCM)
Journal Publications
Zhang, Wei; Fenes, Endre; Ma, Hongfei; Sollund, Erling Olav; Margin, Tigran; Raut, Kumar Ranjan; Chen, De: Promoter doping for tuning the redox behavior of CuCl₂-Al₂O₃-based catalysts in ethylene oxychlorination: Insights from kinetic studies, Chemical Engineering Journal 2023, Volume 47, 144593
Zhang, Wei, Ma, Hongfei, Wang, Yalan; Raut, Kumar Ranjan; Margin, Tigran; Chen, De: Toward Fully-Selective Ethylene Oxychlorination Through Engineering the Cu Oxidation State Spatial Profile, ACS Catalysis 2023, 13, 12, 15107-15114
Hongfei Ma, Xiuxue Zhang, Hao Zhang, Guoyan Ma, Wei Zhang, Zheng Jiang, De Chen: Atomic Cu-N-P-C Active Complex with Integrated Oxidation and Chlorination for Improved Ethylene Oxychlorination, Advanced Science, 2023, Volume 10(8), 2022535
Zhang, Wei; Ma, Hongfei; Wang, Yalan; Regli, Samuel K.; Rønning, Magnus; Rønning, Kumar Ranjan; Margin, Tigran; Chen, De: In situ monitoring of dynamic behavior of La-doped CuCl₂-Al₂O₃ catalyst in ethylene oxychlorination. Journal of Catalysis 2023; Volume 417, 314-322

Oral Presentations
De Chen and Dennis Neu Reaction Network and Kinetic Modelling of By-Product Formation in Ethylene Oxychlorination for CuCl₂-Al₂O₃-Based Catalysts, 28th North American Catalysis Society Meeting, Providence, USA, 2023-06-18 – 2023-06-23
Wei Zhang, Mechanism and Kinetic Studies of Ethylene Oxychlorination to Ethylene Dichloride and Vinyl Chloride, iCSI Annual seminar, Trondheim, Norway, 2023-06-5 - 2023-06-07
De Chen: Main achievements in research and innovation in Industrial Innovation Area 4, ICSI Annual seminar, Trondheim, Norway, 2023-06-5 – 2023-06-07

IIA 5: The Next Step in Direct Activation of Lower Alkanes
Journal Publications
Karoline Kvande, Beatrice Garetto, Gabriele Deplano, Matteo Signorile, Bjørn Gading Solemøl, Sebastian Prodinger, Unni Olsbye, Pablo Beato, Silvia Bordiga, Stian Svelle, and Elisa Borfecchia: Understanding C-H activation in light alkanes over Cu-MOR zeolites by coupled advanced spectroscopy and temperature-programmed reduction experiments, Chemical Science, 2023, 14, 9704-9723
Karoline Kvande, Sebastian Prodinger, Bjørn Gading Solemøl, Silvia Bordiga, Elisa Borfecchia, Unni Olsbye, Pablo Beato, Stian Svelle: Cu-loaded zeolites enable the selective activation of ethane to ethylene at low temperatures and pressure, Chemical Communications, 2023, 59, 6052-6055
Karoline Kvande, Sebastian Prodinger, Fabian Schlimpen, Pablo Beato, Patrick Pole, Stefan Chassarion, Stian Svelle: Copper-zeolites prepared by solid-state ion exchange - characterization and evaluation for the direct conversion of methane to methanol, Topics in Catalysis, 2023, Volume 64, 1406-1417
Prodinger, Sebastian; Capel Berdiell, Izar; Cordero-Lanzac, Tomás; Børsig Brygges, Ole; Solenski, Bjørn; Kvande, Karoline; Bjørn Arstad, Beato, Pablo; Olsbye, Unni; Svelle, Stian: Cation-Induced Speciation of por-SiSize during monodentate zeolite synthesis, Journal of Materials Chemistry A, 2023, 11, 21886-21894
Sun, Xinwei; Valseth, Einar; Ravik, Per Martin; Prodinger, Sebastian; Kalantarpoulos, Georgios; Chatzitokos, Athanasios; Norby, Truls: Surface protonic conductivity in chemisorbed water in porous nanoscopic CeO$_2$. Applied Surface Science 2023, Volume 611, 155590

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

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

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


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

IIAS: Generic Projects for Additional Industrial Synergies
Journal Publications
Ingeborg-Helene Svenum, Marie D. Strømsheim, Jan Knudsen, Hilde J. Venvik: Activity and segregation behavior of Pd$_{50}$Sn$_{50}$ (111) during CO oxidation – An in-situ NAP-XPS investigation. Journal of Catalysis, 2023, Volume 417, 194-201

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

Bjørn Baumgarten: Reducing coking by coupling CO$_2$ Hydrogenation and MTG, iCSI and CATHEX seminar, Trondheim, Norway, 2023-06-5 – 2023-06-07

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

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

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

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

Posters
Svenum, Ingeborg-Helene; Strømsheim, Marie Døvre; Knudsen, Jan; Venvik, Hilde Johannes: Surface reactivity and segregation dynamics of PdAg alloy surfaces by NAP-XPS. Reactions at Surface Active Sites: From Single Atoms and ZD Materials to Electroified Interfaces; 2023-02-12 - 2023-02-17

Svenum, Ingeborg-Helene; Strømsheim, Marie Døvre; Shavorskiy, Andrey; Yu, Junbo; Peters, Thits; Venvik, Hilde Johnson: Surface reactivity and segregation dynamics of PdAg alloy surfaces by NAP-XPS. Chemical Reactions at Surfaces GRC: Reactions at Surface Active Sites: From Single Atoms and ZD Materials to Electroified Interfaces; 2023-02-12 - 2023-02-17

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Antony, Jabin; Villa Gonzalez, Susana; Bandhopadhyay, Sulacic; Yang, Jia; Rønning, Magnus: Silica-modified bisphosphonate nanoparticles for enhanced adsorption and fast solar photocatalytic degradation of methylene blue. Catalysis Today, 2023, Volumes 413-415, 113985

Banan S, Lathifa; Veerapandy, Vasu; Fjellvåg, Helmer; Ponniah, Voyelest; First-Principles Insights into the Relative Stability and Physical and Chemical Properties of MoSe$_2$-ZrO$_2$ intermetallic compounds dispersed on Ce-Zr mixed oxides in the aqueous phase reforming of ethylene glycol. App. Cat. B, 2024, 350, 123904

Copa, A.; González-Vázquez, M.P.; Chen, De; Rubiera, F.; Pevida, C.; Gil, M.V.: Effect of H$_2$S on biogas sorption-enhanced steam reforming using a Pd/Ni-Co catalyst and dolomite as a sorbent. Chemical Engineering Journal, 2023, Volume 476, 146803

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

Choudhary, Mukesh K; Fjellvåg, Helmer; Ponniah, Raviandra: First principle studies on electronic and thermoelectric properties of Pd$_2$Sn$_2$ based multinary Heusler alloys. Computational Materials Science, 2023, Volume 216, 111856

Photo: Magnus Rønning

Bjørn Frederik Baumgarten: Particle size effect for CO$_2$ hydrogenation by In$_2$O$_3$-SrO$_2$ catalysts, 15th EuropaCat 2023 Congress, Prague, Czechia, 2023-08-27 - 2023-09-01

Tina Bergh: Three-dimensional electron microscopy characterisation of silver before and after oxidation of CO, H$_2$ and CH4. 15th EuropaCat 2023 Congress, Prague, Czechia, 2023-08-27 - 2023-09-01
Ivarez Encinas, Oscar Luis; Groven, Anette Synnove; Rout, Kumar Manoj; Bleeker, Edil Andres; Phosphorus deactivation on co-based catalysts for Fischer-Tropsch. Topics in catalysis 2023, Volume 66, 1381-1390

Jing, Li-Jun; Yan, Wei-Qi; Xiao, Han-Jie; Lei, Ming; Cao, Yue-Qiang; Sui, Zhi-Jun; Zhou, Jing-Hong; Zhou, Xing-Gui; Chen, De; Zhou, Yi-An: Interface-enhanced catalytic performance of SO2 supported Cu and Au for dimethyl sulfoxide hydrogenation: A comparative microkinetic analysis. Chemical Engineering Science (CES), 2023, Volume 281, 119176

Li, Ruiyong; Zheng, XiuHui; Wang, Fei; Yan, Hao; Zhao, Xin; Tuo, Yangxiao; Liu, Yibin; Feng, Xiang; Chen, Xiaobo; Chen, De; Yang, Chaohu: Optimizing Mo-C coordination for enhanced low-temperature water-gas shift activity over a-MoC catalysts: An experimental and theoretical study. Chemical Engineering Journal 2023, Volume 474, 154654

Lin, Dong; Feng, Xiang; Zheng, XiuHui; Xu, Yang; Hui; Song, ZhaoNing; Wang, Liang; Shan, HongHong; Xiao, Aofang; Chen, De; Yang, Chaohu: Dimensional Regulation of Titanosilicate by Kinetically Controlled Intergrowth Crystals. Advanced Functional Materials 2023, Volume 33(23), 2301179

Lin, Dong; Mao, Zhiwei; Feng, Xiang; Zhou, Xin; Yan, Hao; Zhu, Huiliang; Liu, Yibin; Chen, Xiaobo; Tuo, Yangxiao; Peng, Cheng; Chen, Xiaobo: Tunable catalytic insights into dehydrogenation of vegetable oils to produce second-generation biodiesel. Fuel 2023, Volume 333 (2), 124616

Lundegaard, Lars Fahel; Capel Berdell, Ivar; König, Nici; Junge, Nicola Haaber; Beato, Pablo; Chernyshov, Dmitry; Svelle, Stian; Wragg, David Stephen: Tracking deactivation of zeolite beta with and without a detailed structure model: XRD analysis and in situ studies. Microporous and Mesoporous Materials, 2023, Volume 366, 112911


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

Ma, Jianyuan; Mahmoudinia, Mehdi; Rout, Kumar Manoj; Bleeker, Edil Andres; High-temperature sulfoxide capture by a Mn-Mo sorbent: An investigation of regeneration conditions and SO2 formation and prevention. Chemical Engineering Science (CES) 2023, Volume 274, 118674

Meng, FanYu; Yan, Hao; Zhao, XiaoQing; Zeng, Jie; Zhou, Xin; Liu, Yibin; Feng, Xiang; Chen, De; Yang, Chaohu: Carbon-based metal-free catalysts for selective oxidation of glycerol to glyoxylic acid. Chemical Engineering Science (CES), 2023, Volume 266, 118394


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


Redekop, Evgeniy; Cordero-Lanzac, Tomáš; Salussola, Davide; Pakle, Anuj; Øren-Bøegegard, Sigurd; Svelle, Stian; Wragg, David Stephen: Tracking deactivation of zeolite beta with and without a detailed structure model: XRD analysis and in situ studies. Microporous and Mesoporous Materials, 2023, Volume 366, 112911

Summa, Paulina; Swirik, Katarzyna; Gopakumar, Jithin; Samojedier, Bogdan; Motak, Monika; Ramage, Magnus; Van Beek, Wouter; Joensen, Finn; Olsbye, Unni: Optimization of Co-Ni-Mg-Al mixed-oxides CO2 methanation catalysts with solution combustion synthesis: On the importance of Ca incorporation and basicity. Applied Materials, 2023, Volume 33, 146-158

Tezel, Elif; Sannes, Dog Kristian; Svelle, Stian; Zielińska, Petra Agata; Olsbye, Unni: Direct CO2 to methanol reduction on Zr2Mo5OF17 based composite catalysts: A critical review. Materials Advances, 2023, 4, 5479-5495

Ticoli, Pierfrancesco; Salussola, Davide; Arie, Alessia; Morandi, Sara; Barfeczchib, Elisa; Ramirez, Adrian; Cordero-Lanzac, Tomás; Gascon, Jorge; Olsbye, Unni; Joensen, Finn; Bordiga, Silvia: From Lab to Technical CO2 Hydrogenation Catalysis: Understanding PdO Decomposition. Applied Materials & Interfaces, 2023, Volume 15(4), 5218-5228

Tuo, Yongxiao; Liu, Wanli; Lu, Qing; Wang, Xianzhao; Luo, Jiaobin; Wang, Shutaow; Zhou; Yan, Min; Sun, Xiaohui; Feng, Xiang; Wu, Mingbo; Chen, De; Zhang, Jun: Atomic Zn-Doping Induced Sabatier Optimum in Ni2Zn2O5 Catalyst for CO2 Electroreduction at Industrial-Level Current Densities, Small, 2023, Early version 2306945

Tuo, Yongxiao; Meng, Yang; Lu, Qing; Wang, Qing; Jia, Furong; Zhou; Yan; Feng, Xiang; Zhang, Jun; Duan, Xuezh; Chen, De: Taming Pt Sd state occupancy via Pt-O-Mn electronic link- age for enhanced deuteration activity. ACHE Journal, 2023, Volume 69(9), e18149

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Yan, Hao; Liu, Bowen; Zhou, Xin; Meng, FanYu; Zhao, Mingyue; Pan, Yue; Li, Jie; Wu, Yining; Zhao, Hui; Liu, Yibin; Chen, Xiaobo; Li, Lina; Feng, Xiang; Chen, De; Shan, HongHong; Yang, Chaohu; Yan, Ning: Enhancing polyolsulph-4 or cascade oxidation to formic acid with defect rich Ni-Mo2 nature catalysts. Nature Communications, 2023, Volume 14 (1), 4509

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

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

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

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

Ask Lysne: Hydrotalcite-Derived Nickel-Cobalt Catalysts for CO₂ Valorization, iCSI and CATHEX seminar, Trondheim 2023-06-05 - 2023-06-08

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

XRD. NKS-FUM 2023; 2023-02-13 - 2023-02-14

Anja Olafsen; Fjellvåg, Helmer: Tracing the (De)sodiation Parameter Effects, 15th EuropaCat 2023 Congress, Prague, Czechia, 2023-08-27 - 2023-09-01

Ingeborg-Helene Syvum: Understanding the interaction of CH₄/CH₃Cl with Ce-based surfaces, 15th EuropaCat 2023 Congress, Prague, Czechia, 2023-08-27 - 2023-09-01

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

Tomas Cordero-Lanzac, Adiran Ramirez, Marta Cruz-Fernandez, Hans-Jörg Zander, Finn Joensen, Andreas Meiswinkel, Jorge Gacitan and Unni Olsbye: Kinetic Model, Process Design and LCA of a CO₂ Valorization Plant to Produce Light Hydrocarbon Using a Pd/ZrO₂ + SAPO-34 Catalyst, 28th North American Catalysis Society Meeting, Providence, USA, 2023-06-18 - 2023-06-23

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

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

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

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

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

Agnieszka Seremak: Theoretical study of local and global defects in UiO-type metal-organic frameworks: selective, active and stable catalysts for hydrogenation reactions, 15th EuropaCat 2023 Congress, Prague, Czechia, 2023-08-27 - 2023-09-01

Rama, Raquel J.; Nova, Ainara; Olsbye, Unni; Synthesis of linker-based bifunctional ligands for UO₂-67 metal-organic frameworks. 6th EuChemS Inorganic Chemistry Conference; 2023-09-03 - 2023-09-07

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

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Acknowledgements

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

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

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Dr. Anne Hoff and Prof. Hilde Johnsen Venvik, NTNU